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Revised Robust Summaries for Ketone Bottoms (KB4/KB3)

CAS No. 68990-20-5

Eastman Chemical Company

Registration Number

Submitted to the EPA under the HPV Challenge Program by:

Eastman Chemical Company
100 North Eastman Road
Kingsport, TN 37662
Phone: 423-229-5208
Fax: 423-224-0208

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Robust Summaries for Ketone Bottoms (KB4)

The evaluation of the quality of the following data uses a systematic approach described by Klimisch [Klimisch *et al*., 1996]. Based on criteria relating to international testing standards for categorizing data reliability, four reliability categories have been established. The following categories are:

- Reliability code 1.Reliable without restrictions
- Reliability code 2.Reliable with restrictions
- Reliability code 3.Not reliable
- Reliability code 4.Not assignable

1 CHEMICAL AND PHYSICAL PROPERTIES

1.1 Melting Point

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Melting Point	-8 °C
Decomposition	
Sublimation	
Remarks for Results	

Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.
CAS	925-78-0
Substance Name	3-Nonanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Melting Point	-18.94 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Syracuse Research Corporation (SRC) Private communication to FMA.
CAS	4485-09-0
Substance Name	4-Nonanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	

Melting Point	-5.85 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1976
Remarks for Test Conditions	
Melting Point	-5.9 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Alarie Y. *et al*. (1995) MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for substance	
Method/guideline	Experimental

GLP	Ambiguous
Year	1994
Remarks for Test Conditions	
Melting Point	-4.8 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Clayton J. D. and Clayton F. E. (1994) Patty's Industrial Hygiene and Toxicology, 4th Ed., Ketones. Eds Topping C. D., Morgott D. a., David R. M., and O'Donoghue J. L., pp 1749-1750.

CAS	693-54-9
Substance Name	2-Decanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Melting Point	14 °C; freezing point 3.1 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	928-80-3
Substance Name	3-Decanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Melting Point	2.5 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	928-80-3
Substance Name	3-Decanone
Remarks for substance	Same predicted data for 2-, 4-, or 5-decanone.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Melting Point	5.92 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	

Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	624-16-8
Substance Name	4-Decanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Melting Point	-9 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1984
Remarks for Test Conditions	
Melting Point	15 °C
Decomposition	

Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Perry R. H. and Green D (1984) MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Melting Point	12.1 - 12.7 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	
Method/guideline	Calculated
GLP	

Year	
Remarks for Test Conditions	
Melting Point	10 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	2216-87-7
Substance Name	3-Undecanone
Remarks for substance	Same predicted data for 2-, 4-, 5-, or 6-undecanone
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Melting Point	17.15 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	14476-37-0
Substance Name	4-Undecanone

Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Melting Point	4.5 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	927-49-1
Substance Name	6-Undecanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Melting Point	15 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc.,

	Boca Raton, FL.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1984
Remarks for Test Conditions	
Melting Point	21 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Perry R. H. and Green D (1984) MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for substance	Same predicted data for 3-, 4-, 5-, or 6-dodecanone
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Melting Point	27.86 °C
Decomposition	
Sublimation	
Remarks for Results	

Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	1534-27-6
Substance Name	3-Dodecanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Melting Point	19 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.
CAS	6137-26-4
Substance Name	4-Dodecanone
Remarks for substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Melting Point	10 °C

Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Melting Point	-1.09 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for substance	Same predicted data for 2,6- or 2,4-dimethylcyclohexanone
Method/guideline	Calculated
GLP	

Year	
Remarks for Test Conditions	
Melting Point	-13.73 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for substance	Data for isomer, 5-methyl-3-heptanone isomer
Method/guideline	Experimental
GLP	Ambiguous
Year	1994
Remarks for Test Conditions	
Melting Point	-56.7 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Clayton J. D. and Clayton F. E. (1994) Patty's Industrial Hygiene and Toxicology, 4th Ed., Ketones. Eds Topping C. D., Morgott D. a., David R. M., and O'Donoghue J. L., pp 1749-1750.

CAS	2345-28-0 2

Substance Name	2-Pentadecanone
Remarks for substance	Same predicted data for 2-, 6-, 8-pentadecanone
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Melting Point	46.2 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS Numerical	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Melting Point	-7.03 °C
Decomposition	
Sublimation	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection

	Agency.
CAS Numerical	67662-98-0
Substance Name	3-Methyl-5-propylcyclohexanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Melting Point	9.03 °C
Decomposition	
Sublimation	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection

1.2 Boiling Point

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	195.3 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Boiling Point	192 °C
Pressure	742 mm Hg

Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Fragrance Materials Association (FMA) Private communication.

CAS	925-78-0
Substance Name	3-Nonanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Boiling Point	187 °C
Pressure	751 mm
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	925-78-0
Substance Name	3-Nonanone
Remarks for Substance	
Method/guideline	Experimental

GLP	Ambiguous
Year	
Remarks for Test Conditions	
Boiling Point	190 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Fragrance Materials Association (FMA) Private communication.

CAS	4485-09-0
Substance Name	4-Nonanone
Remarks for Substance	Same predicted data for 2-, 3-, 4-, 5-nonanone.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Boiling Point	184.65 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1994
Remarks for Test Conditions	
Boiling Point	188.4 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Clayton J. D. and Clayton F. E. (1994) Patty's Industrial Hygiene and Toxicology, 4th Ed., Ketones. Eds Topping C. D., Morgott D. A., David R. M., and O'Donoghue J. L., pp 1749-1750.

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	186-187 °C
Pressure	
Pressure Unit	

Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	211; 215.5 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.
CAS	928-80-3
Substance Name	3-Decanone
Remarks for Substance	Same predicted data for 2-, 3-, 4-, 5-decanone.
Method/guideline	Calculated

GLP	
Year	
Remarks for Test Conditions	
Boiling Point	204.79 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	624-16-8
Substance Name	4-Decanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	206 - 207 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	228 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	231 °C
Pressure	
Pressure Unit	
Decomposition	

Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Fragrance Materials Association (FMA) Private communication.

CAS	2216-87-7
Substance Name	3-Undecanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Boiling Point	227 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	2216-87-7
Substance Name	3-Undecanone
Remarks for Substance	Same predicted data for 2-, 3-, 4-, 5-, 6-undecanone.
Method/guideline	Calculated
GLP	
Year	

Remarks for Test Conditions	
Boiling Point	224.03 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	927-49-1
Substance Name	6-Undecanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	228 °C (cor.)
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.
CAS	1534-27-6

Substance Name	3-Dodecanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	234 °C
Pressure	18 mm Hg
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1984
Remarks for Test Conditions	
Boiling Point	246.5 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	

Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Perry R. H. and Green D. (1984) MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Same predicted data for 2-, 3-, 4-, 5-, 6-dodecanone.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Boiling Point	242.37 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	179 °C

Pressure	748 mmHg
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	178-179 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone

Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	174 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	823-55-2
Substance Name	2,4-Dimethylcyclohexanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	171 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.

Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	
Method/guideline	Experimental
GLP	Ambiguous
Year	1960
Remarks for Test Conditions	
Boiling Point	171 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	CRC Handbook of Chemistry and Physics (2000) 82nd edition, David R. Lide, editor, The Chemical Rubber Co. Press, Inc., Boca Raton, FL.

CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	
Method/guideline	Experimental
GLP	
Year	
Remarks for Test Conditions	
Boiling Point	294 °C

Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Boiling Point	291.96 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	5440-89-1
Substance Name	4-Ethyl-2-nonanone
Remarks for Substance	

Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Boiling Point	214.54 °C
Pressure	
Pressure Unit	
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	67662-98-0
Substance Name	3-Mthyl-5-propylcyclohexanone
Remarks for Substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Boiling Point	224.46 °C
Pressure	
Pressure Unit	
Decomposition	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

1.3 Vapor Pressure

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for substance	
Method/guideline	Measured
GLP	Ambiguous
Year	
Remarks for Test Conditions	
Vapor Pressure	0.30 mm Hg
Temperature	20 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Fragrance Materials Association (FMA) Private communication. Unpublished report.

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for substance	
Method/guideline	Measured
GLP	Ambiguous
Year	1976
Remarks for Test Conditions	
Vapor Pressure	0.642 mm Hg
Temperature	25 °C

Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Ohe S. (1976) MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	820-29-1
Substance Name	2-Nonanone
Remarks for substance	Calculated vapor pressure values for 2-,3-, 4-, or 5-nonanone are equivalent.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	0.933 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	925-78-0
Substance Name	3-Nonanone
Remarks for substance	
Method/guideline	Measured
GLP	Ambiguous
Year	

Remarks for Test Conditions	
Vapor Pressure	0.83 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Syracuse Research Corporation (SRC)

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for substance	
Method/guideline	Measured
GLP	Ambiguous
Year	1995
Remarks for Test Conditions	
Vapor Pressure	0.552 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Alarie Y. *et al*. (1995) MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	693-54-9
Substance Name	2-Decanone
Remarks for substance	

Method/guideline	Measured
GLP	Ambiguous
Year	1995
Remarks for Test Conditions	
Vapor Pressure	0.269 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Perry R. H. and Green D (1984) MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	693-54-9
Substance Name	2-Decanone
Remarks for substance	Calculated vapor pressure values for 2-, 3-, 4-, or 5-decanone are equivalent.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	0.449 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	
Method/guideline	Measured
GLP	Ambiguous
Year	1984
Remarks for Test Conditions	
Vapor Pressure	0.0414mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Perry R. H. and Green D (1984) MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	0.03mm Hg
Temperature	20 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.

Remarks for Data Reliability	Code 4. Calculated.
References	Fragrance Materials Association (FMA) Private communication. Unpublished report.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	Calculated vapor pressure values for 2-, 3-, 4-, 5- or 6-undecanone are equivalent.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	0.14mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	927-49-1
Substance Name	6-Undecanone
Remarks for substance	
Method/guideline	Measured
GLP	Ambiguous
Year	1975
Remarks for Test Conditions	
Vapor Pressure	0.05 mm Hg
Temperature	20 °C
Decomposition	

Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Engineering Sciences Unit (1975) MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for substance	
Method/guideline	Measured
GLP	Ambiguous
Year	1984
Remarks for Test Conditions	
Vapor Pressure	0.0206 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Perry R. H. and Green D (1984) MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	1534-27-6
Substance Name	3-Dodecanone
Remarks for substance	Calculated vapor pressure values for 2-, 3-, 4-, or 5-dodecanone are equivalent.
Method/guideline	Calculated
GLP	
Year	

Remarks for Test Conditions	
Vapor Pressure	0.065 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	1.32 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for substance	

Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	1.04 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	1.66 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	823-55-2
Substance Name	2,4-Dimethylcyclohexanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	1.04 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for substance	
Method/guideline	Calculated vapour pressure for 2-, 6-, or8-pentadecanone are equivalent
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	0.0036 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.

Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	0.284 mm Hg
Temperature	25 °C
Decomposition	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.
CAS	67662-96-0
Substance Name	3-Methyl-5-propylcyclohexanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Vapor Pressure	0.158 mm Hg
Temperature	25 °C
Decomposition	

Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	MPBPVP EPI Suite (2000) US Environmental Protection Agency.

1.4 n-Octanol/Water Partition Coefficients

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for substance	
Method/guideline	GC method
GLP	
Year	1986
Remarks for Test Conditions	Analysis was carried out using gas chromatograph equipped with flame ionization detector and PEG 20M glass column. Column temperature was 155 C. Volume for partitioning was 8.0 ml water and 0.01 ml octanol. Values are means of triplicate runs.
Log Pow	3.14
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Tanii H., Tsuji H., Hashimoto K. (1986) Structure-toxicity relationships of monoketones. Toxicology Letters 30, 13-17.

CAS	821-55-6
Substance Name	2-Nonanone

Remarks for substance	Calculated values of log Kow for 2-, 3-, 4-, or 5-nonanone are equivalent.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	2.71
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for substance	
Method/guideline	Experimental
GLP	
Year	1989
Remarks for Test Conditions	
Log Pow	3.06
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Hansch C., Kim D., Leo A. J., Novellino E., Silipo C., and Vittoria A. (1989). Toward a comparative toxicology of organic compounds. Critical Reviews in Toxicology 19, 185-226.

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for substance	
Method/guideline	Experimental
GLP	
Year	1967
Remarks for Test Conditions	Partition coefficient was calculated from the molecular fragment constant method.
Log Pow	2.79
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Hansch C., Quinlan J. E., and Lawrence G. L. (1967) The linear free-energy relationship between partition coefficients and aqueous solubility of organic liquids. Journal of Organic Chemistry, 33, 347-351.

CAS	502-56-7
Substance Name	5-Nonanone
Remarks for substance	
Method/guideline	Experimental
GLP	
Year	1994
Remarks for Test Conditions	
Log Pow	2.88
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.

References	Abraham M. H. (1994) KOWWIN EPI Suite (2000) US Environmental Protection Agency.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for substance	
Method/guideline	Experimental
GLP	
Year	1989
Remarks for Test Conditions	
Log Pow	3.60
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Hansch C., Kim D., Leo A. J., Novellino E., Silipo C., and Vittoria A. (1989). Toward a comparative toxicology of organic compounds. Critical Reviews in Toxicology 19, 185-226.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for substance	
Method/guideline	GC method
GLP	
Year	1986
Remarks for Test Conditions	Analysis was carried out using gas chromatograph equipped with flame ionization detector and SE 30 glass column. Column temperature was 155 C. Volume for partitioning was 20.0 ml water and 0.03 ml octanol. Values are means of triplicate runs.
Log Pow	3.73
Temperature	25 °C
Remarks for Results	

Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Tanii H., Tsuji H., Hashimoto K. (1986) Structure-toxicity relationships of monoketones. Toxicology Letters 30, 13-17.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for substance	Calculated values of log Kow for 2-, 3-, 4-, or 5-decanone are equivalent.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	3.21
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	
Method/guideline	GC method
GLP	
Year	1986
Remarks for Test Conditions	Analysis was carried out using gas chromatograph equipped with flame ionization detector and SE 30 glass column. Column temperature was 170 C. Volume for partitioning was 16.0 ml water and 0.01 ml octanol. Values are means of triplicate runs.
Log Pow	4.09

Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Tanii H., Tsuji H., Hashimoto K. (1986) Structure-toxicity relationships of monoketones. Toxicology Letters 30, 13-17.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for substance	Calculated values of log Kow for 2-, 3-, 4-, 5-, or 6-undecanone are equivalent.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	3.69
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for substance	Data are for higher homologue, 7-tridecanone
Method/guideline	Experimental
GLP	
Year	1979
Remarks for Test Conditions	Partition coefficient calculated from molecular fragment constant method.

Log Pow	5.17
Temperature	25 °C
Remarks for Results	Partition coefficient of 2-dodecanone estimated to be 4.6
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Hansch C. and Leo A. (1979) Substituent constants for correlation analysis in chemistry and biology. John Wiley & Sons, New York, 339p.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for substance	Calculated values of log Kow for 2-, 3-, 4-, 5-, or 6-dodecanone are equivalent.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	4.18
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for substance	Calculated values of log Kow for 3,3- 2,3-, 2,6-, or 2,4-dimethylcyclohexanone are equivalent.
Method/guideline	Calculated
GLP	

Year	
Remarks for Test Conditions	
Log Pow	1.98
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for substance	Data for homologue, 2-octanone
Method/guideline	Experimental
GLP	
Year	1989
Remarks for Test Conditions	
Log Pow	2.52
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Hansch C., Kim D., Leo A. J., Novellino E., Silipo C., and Vittoria A. (1989) Toward a comparative toxicology of organic compounds. Critical Reviews in Toxicology, 19, 185-226.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for substance	Data for homologue, 2-octanone
Method/guideline	Experimental

GLP	
Year	1979
Remarks for Test Conditions	Partition coefficient calculated from molecular fragment constant method.
Log Pow	2.46
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Hansch C. and Leo A. (1979) Substituent constants for correlation analysis in chemistry and biology. John Wiley & Sons, New York, 339p.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	2.42
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	2345-28-0
Substance Name	2-Pentadecanone

Remarks for substance	Calculated values for 2-, 6-, or 8-pentadecanone are equivalent
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	5.66
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	3.62
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	67662-98-0

Substance Name	3-methyl-5-propylcyclohexanone
Remarks for substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Log Pow	2.94
Temperature	25 °C
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	KOWWIN EPI Suite (2000) US Environmental Protection Agency.

1.5 Water Solubility

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data for 2-, 3-, 4-, and 5-nonanone are shown.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Value (mg/L) at temperature	170.6 mg/L for 2-nonanone, 396.1 mg/L for 3-nonanone, 284.4 mg/L for 4- or 5-nonanone
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	

Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.
CAS	502-56-7
Substance Name	5-Nonanone
Remarks for Substance	
Method/guideline	Experimental
GLP	No
Year	1947
Remarks for Test Conditions	
Value (mg/L) at temperature	376 mg/L at 25 °C
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	Data cited in Hansch *et al.,* 1967
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Only short abstract available.
References	Palit S. R. (1947) Journal of Physical Chemistry, 51, 827.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Data for 2-, 3-, 4-, and 5-decanone are shown.
Method/guideline	Calculated
GLP	
Year	

Remarks for Test Conditions	
Value (mg/L) at temperature	46.4 mg/L for 2-decanone, 131 mg/L for 3-, 4- or 5-decanone
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Data for 2-, 3-, 4-, 5-, and 6-undecanone are shown.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Value (mg/L) at temperature	19.7 mg/L for 2-undecanone, 42.9 mg/L for 3-, 4-, 5-, or 6-undecanone
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Data for 2-, 3-, 4-, 5-, and 6-dodecanone are shown.
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Value (mg/L) at temperature	14 mg/L for 2-, 3-, 4-, 5-, or 6-dodecanone
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Value (mg/L) at temperature	1874 mg/L at 25 °C
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	

Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Value (mg/L) at temperature	1371 mg/L at 25 °C
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.
CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	Values for 2-, 6-, or 8-pentadecanone are equivalent
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	

Value (mg/L) at temperature	0.486 mg/L at 25 °C
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.

CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for Substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Value (mg/L) at temperature	49.63 mg/L at 25 °C
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.

CAS	67662-98-0
Substance Name	3-Methyl-5-propylcyclohexanone

Remarks for Substance	
Method/guideline	Calculated
GLP	
Year	
Remarks for Test Conditions	
Value (mg/L) at temperature	222.7 mg/L at 25 °C
Description of Solubility	
pH value and concentration at temp	
pKa value at 25 Celsius	
Remarks for Results	
Conclusion Remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	WSKOWWIN EPI Suite (2000) U.S. Environmental Protection Agency.

2 ENVIRONMENTAL FATE AND PATHWAYS

2.1 Photodegradation

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Assay: 99%
Method/guideline	Flash photolysis resonance fluorescence
Test Type	Hydroxyl radical reaction
GLP	No
Year	1987
Light Source	Nitrogen-pulsed discharge lamp
Light Spectrum (nm)	165 nm
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	Hydroxyl radicals were produced by ultraviolet flash photolysis of water at 0.1 Torr. Radical concentrations were monitored as a function of time by fluorescence from an OH microwave resonance lamp. Hydroxyl radical concentrations were maintained between 10 exp 10 to 10 exp 11 molecules/cm3. Concentration anticipated to be sufficient to assure pseudo-first order kinetics for radical decay.
Concentration of Substance	
Temperature	296K
Direct photolysis	
Halflife t1/2	6.3 hours at atmospheric
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=122 x 10exp-13 cu cm/molecule.sec

Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	Material is expected to undergo rapid degradation in the atmosphere.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Wallington T. J. and Kurylo, M. J. (1987) Flash photolysis resonance fluorescence investigation of the gas-phase reaction of OH radicals with a series of aliphatic ketones over the temperature range 240-444 K. Journal of Chemical Physics, 91, 5050-5054.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data for 2-, 3-, 4-, and 5-nonanone are shown.
Method/guideline	Calculation
Test Type	AOPWIN
GLP	
Year	2000
Light Source	
Light Spectrum (nm)	
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	t1/2=11.67 hrs for 2-nonanone, 11.979 hrs for 3-nonanone, 10.073 hrs for 4-nonanone, and 9.639 hrs for 5-nonanone
Degradation % after	
Quantum yield	
Indirect photolysis	

Sensitizer	
Concentration of sensitizer	
Rate constant	k=10.99 x 10exp-12 cu cm/molecule-sec for 2-nonanone, 10.71 x 10 exp-12 cu cm/molecule-sec for 3-nonanone, 12.74 x 10exp-12 cu cm/molecule-sec for 4-nonanone, 13.311 x 10exp-12 cu cm/molecule-sec for 5-nonanone
Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Assay: 98%
Method/guideline	Flash photolysis resonance fluorescence
Test Type	Hydroxyl radical reaction
GLP	No
Year	1987
Light Source	Nitrogen-pulsed discharge lamp
Light Spectrum (nm)	165 nm
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	Hydroxyl radicals were produced by ultraviolet flash photolysis of water at 0.1 Torr. Radical concentrations were monitored as a function of time by fluorescence from an OH microwave resonance lamp. Hydroxyl radical concentrations were maintained between 10 exp 10 to 10 exp 11 molecules/cm3. Concentration anticipated to be sufficient to assure pseudo-first order kinetics for radical decay.
Concentration of Substance	
Temperature	296K

Direct photolysis	
Halflife t1/2	6.8 hours at atmospheric
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=132 x 10exp-13 cu cm/molecule.sec
Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	Material is expected to undergo rapid degradation in the atmosphere
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Wallington T. J. and Kurylo, M. J. (1987) Flash photolysis resonance fluorescence investigation of the gas-phase reaction of OH radicals with a series of aliphatic ketones over the temperature range 240-444 K. Journal of Chemical Physics, 91, 5050-5054.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Data for 2-, 3-, 4-, and 5-decanone are shown.
Method/guideline	Calculation
Test Type	AOPWIN
GLP	
Year	2000
Light Source	
Light Spectrum (nm)	
Relative Intensity	
Spectrum of Substance	

Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	t1/2=10.34 hrs for 2-decanone, 10.58 hrs for 3-decanone, 9.067 hrs for 4-decanone, and 8.714 hrs for 5-decanone
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=12.40 x 10exp-12 cu cm/molecule-sec for 2-decanone, 12.128 x 10 exp-12 cu cm/molecule-sec for 3-decanone, 14.156 x 10exp-12 cu cm/molecule-sec for 4-decanone, 14.73 x 10exp-12 cu cm/molecule-sec for 5-decanone
Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Data for 2-, 3-, 4-, 5-, and 6-undecanone are shown.
Method/guideline	Calculation
Test Type	AOPWIN
GLP	
Year	2000
Light Source	
Light Spectrum (nm)	

Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	t1/2=9.28 hrs for 2-undecanone, 9.48 hrs for 3-undecanone, 8.244 hrs for 4-undecanone, and 7.951 hrs for 5- and 6-undecanone
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=13.82 x 10exp-12 cu cm/molecule-sec for 2-undecanone, 13.54 x 10 exp-12 cu cm/molecule-sec for 3-undecanone, 15.568 x 10exp-12 cu cm/molecule-sec for 4-undecanone, 16.14 x 10exp-12 cu cm/molecule-sec for 5- and 6-undecanone
Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Data for 2-, 3-, 4-, 5-, and 6-dodecanone are shown.
Method/guideline	Calculation
Test Type	AOPWIN

GLP	
Year	2000
Light Source	
Light Spectrum (nm)	
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	t1/2=8.423 hrs for 2-dodecanone, 8.583 hrs for 3-dodecanone, 7.558 hrs for 4-dodecanone, and 7.31 hrs for 5- and 6-dodecanone
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=15.23 x 10exp-12 cu cm/molecule-sec for 2-dodecanone, 14.95 x 10 exp-12 cu cm/molecule-sec for 3-dodecanone, 16.98 x 10exp-12 cu cm/molecule-sec for 4-dodecanone, 17.55 x 10exp-12 cu cm/molecule-sec for 5- and 6-dodecanone
Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	2979-19-3

Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data for 3,3-, 2,3-, 2,6-, and 2,4-dimethylcyclohexanone are shown.
Method/guideline	Calculation
Test Type	AOPWIN
GLP	
Year	2000
Light Source	
Light Spectrum (nm)	
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	t1/2=16.142 hrs for 3,3-isomer, 6.921 hrs for 2,3- isomer, 8.549 hrs for 2,6- isomer, and 8.419 hrs for 2,4- isomer
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=9.7512 x 10exp-12 cu cm/molecule-sec for 3,3- isomer, 18.548 x10 exp-12 cu cm/molecule-sec for 2,3-isomer, 15.014 x 10exp-12 cu cm/molecule-sec for 2,6-isomer, and 15.248 x 10exp-12 cu cm/molecule-sec for 2,4-isomer
Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Assay: 99%. Data are for isomer 2-octanone.
Method/guideline	Flash photolysis resonance fluorescence
Test Type	Hydroxyl radical reaction
GLP	No
Year	1987
Light Source	Nitrogen-pulsed discharge lamp
Light Spectrum (nm)	165 nm
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	Hydroxyl radicals were produced by ultraviolet flash photolysis of water at 0.1 Torr. Radical concentrations were monitored as a function of time by fluorescence from an OH microwave resonance lamp. Hydroxyl radical concentrations were maintained between 10 exp 10 to 10 exp 11 molecules/cm3. Concentration anticipated to be sufficient to assure pseudo-first order kinetics for radical decay.
Concentration of Substance	
Temperature	296K
Direct photolysis	
Halflife t1/2	5.8 hours at atmospheric
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=110 x 10exp-13 cu cm/molecule.sec
Degradation %after	
Breakdown products	
Remarks field for results	
Conclusion remarks	Material is expected to undergo rapid degradation in the atmosphere

Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Wallington T. J. and Kurylo, M. J. (1987) Flash photolysis resonance fluorescence investigation of the gas-phase reaction of OH radicals with a series of aliphatic ketones over the temperature range 240-444 K. Journal of Chemical Physics, 91, 5050-5054.
CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	Values for 2-, 6-, or 8-pentadecanoneare equivalent.
Method/guideline	Calculated
Test Type	AOPWIN
GLP	
Year	2000
Light Source	
Light Spectrum (nm)	
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	6.99 hours at atmospheric
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=19.47 x 10exp-13 cu cm/molecule.sec
Degradation %after	
Breakdown products	

Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.
CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for Substance	
Method/guideline	Calculated
Test Type	AOPWIN
GLP	
Year	2000
Light Source	
Light Spectrum (nm)	
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	8.844 hours at atmospheric
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=1.451 x 10exp-13 cu cm/molecule.sec
Degradation %after	
Breakdown products	

Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.
CAS	67662-98-0
Substance Name	3-Methyl-5-propylcyclohexanone
Remarks for Substance	
Method/guideline	Calculated
Test Type	AOPWIN
GLP	
Year	2000
Light Source	
Light Spectrum (nm)	
Relative Intensity	
Spectrum of Substance	
Remarks for Test Conditions	
Concentration of Substance	
Temperature	
Direct photolysis	
Halflife t1/2	4.79 hours at atmospheric
Degradation % after	
Quantum yield	
Indirect photolysis	
Sensitizer	
Concentration of sensitizer	
Rate constant	k=4.792 x 10exp-13 cu cm/molecule.sec
Degradation %after	
Breakdown products	

Remarks field for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	AOPWIN EPI Suite (2000) US Environmental Protection Agency.

2.2 Biodegradation

CAS	123-18-2
Substance Name	2,6,8-Trimethyl-4-nonanone (IBHK)
Remarks for Substance	Assay: 91+%
Method	OECD TG-301D
Test Type	Ready Biodegradability by the Closed Bottle Method
GLP	Yes
Year	2004
Contact time (units)	28 days
Innoculum	Activated sludge was collected from the City of Midland Municipal Wastewater Treatment Plant, Midland, Michigan
Remarks for Test Conditions	This study investigated the biodegradation of the test substance in closed bottles under aerobic conditions for 28 days. Due to the limited solubility, 21.5 uL (17.0 rag) IBHK was added directly to 2 L of inoculated mineral media and stirred to prepare the test suspensions. The 2 L of inoculated mineral media and IBHK was then combined with 6 liters of inoculated mineral media for a final concentration of 2.14 mg IBHK/L and dispensed into 18-BOD bottles (300 mL): Negative controls (blank), toxicity controls and reference controls (sodium benzoate: 4.02 mg/L) were also prepared, at replicate numbers of 18, 6 and 6, respectively. The flasks were statically incubated at 20.1¢0.1°C in the dark. Oxygen in the sealed head.space above each test substance solution was measured on the following study days: 0, 3, 5, 7, 11, 14, 17, 21 and 28. Oxygen from the toxicity and reference controls was measured on study days: 0, 3, 7 and 14.
Degradation % after time	44.7% (greater than 60% by Day 14)
Results	

Incubation Time (days)	%Biodegradation	Positive Controls
0	0	0
3	3.2 ±0.2	68.3 ±1.9
5	3.6 ±0.0	
7	3.3 ±0.2	78.5 ±1.0
11	7.8±2.3	
14	19.9 ±2.3	82.3 ±0.5
17	36.4 ±1.9	
21	41.2 ±0.4	
28	44.7 ± 0.3	

Kinetic	
Time required for 10% degradation	12 days
10 day window criteria	No
Total degradation	44.7%
Classification	Readily biodegradable
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	According to the OECD guidelines is not considered readily biodegradable.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Dow Chemical (2004) Ready Biodegradability of 2,6,8-trimethyl-4-nonanone by the Closed Bottle Method. Unpublished Report.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data are for homologue, 2-heptanone; purity 99.7%
Method	Method C.5.: "Degradation, Biochemical Oxygen Demand" Method is similar to OECD: TG-301C: Modified MITI Test.
Test Type	Biochemical Oxygen Demand (BOD)
GLP	Yes
Year	1997
Contact time (units)	

Innoculum	
Remarks for Test Conditions	BOD was determined after 5 and 20 days. The 20-day value was performed in duplicate. The microbial innoculum was prepared from a mixed liquor seed water sample obtained from Kings Landing water treatment facility. The concentration of the innoculum for the study was prepared a 100 ml of the seed water to 2 liters of distilled water. The initial concentration of the test substance was 1 ml of test substance to 1 liter or reagent water.
Degradation % after time	
Results	BOD was 1.77 g BOD/g of test substance BOD20 was 2.00 g BOD/g of test substance
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	Readily biodegradable
Breakdown products (transient or stable)	
Remarks fields for results	The BOD 20 value was a mean of two replicates.
Conclusion remarks	The substance is considered to be "Readily Biodegradable" based on a BOD5/COD ratio greater than 0.5 (1.77/2.42 = 0.73).
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Eastman Chemical Co. (1997b) Biochemical Oxygen Demand Determination; Environmental Analytical Services, Chemicals Quality Services Division, Eastman Kodak Company, Rochester, NY; Report No. COD-00589. July 24, 1997.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data are for homologue, 2-heptanone; purity 99.7%.
Method	Method C.6, Degradation, Chemical Oxygen Demand, Official Journal of European Communities, No. 383A/227, 9/12/92
Test Type	Chemical Oxygen Demand (COD)
GLP	Yes
Year	1997

Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	2.42 g COD/g of test substance
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	Readily biodegradable
Breakdown products (transient or stable)	
Remarks fields for results	The value is a mean of three replicates.
Conclusion remarks	The substance is concluded to be readily biodegradable based on COD criteria.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Eastman Chemical Co. (1997a) Chemical Oxygen Demand Determination; Environmental Analytical Services, Chemicals Quality Services division, Eastman Kodak Company, Rochester, NY; Report No. COD-00590. July 24, 1997.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	The model predictions for 2-, 3-, 4-, or 5-nonanone are similar.
Method	Calculated
Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	

Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks and days to weeks, respectively.
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	The model predictions for 2-, 3-, 4-, or 5-decanone are similar.
Method	Calculated
Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks and days to weeks, respectively.
Kinetic	
Time required for 10%	

degradation	
10 day window criteria	
Total degradation	
Classification	
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	The model predictions for 2-, 3-, 4-, 5-, or 6-undecanone are similar.
Method	Calculated
Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks and days to weeks, respectively.
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	

Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	The model predictions for 2-, 3-, 4-, 5-, or 6-dodecanone are similar.
Method	Calculated
Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks and days to weeks, respectively.
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.

Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	The model predictions for 2,3-, 3,3-, 2,4-, or 2, 6-dimethylcyclohexanone are similar.
Method	Calculated
Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks to months and weeks, respectively.
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for structurally related substance 5-methyl-2-hexanone, purity 99.3%.
Method	OECD TG-301D
Test Type	Ready Biodegradability by the Closed Bottle Method
GLP	Yes
Year	2001
Contact time (units)	28 days
Innoculum	Activated sludge
Remarks for Test Conditions	Benzoic acid at 10 mg/L was used as a reference control. The test material was assessed at a nominal concentration of 2.5 mg/L. Test vessels of 300 ml BOD bottles were prepared per treatment (reference, test substance and innoculum blank), two each for Day 0 and three per sampling interval (Day 7, 14, 21, 28). After the bottles were filled they were closed and wrapped in tin foil.
Degradation % after time	67% (greater than 60% by Day 14)
Results	
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	Readily biodegradable
Breakdown products (transient or stable)	
Remarks fields for results	Benzoic acid reference was degraded 72%. The temperature of the environment ranged from 20-22 deg C. Dissolved oxygen concentrations in the control blank ranged from 8.7 mg/L on Day 0 to 7.1 mg/L on Day 28. The protocol stated that oxygen depletion in the controls should not exceed a loss of 1.5 mg/L before Day 28; however, the loss was 1.6 mg/L. This protocol deviation was viewed as minor and does not affect the overall conclusion as it occurred well after Day 14 when the material had already met the readily biodegradable pass level of greater than 60%.
Conclusion remarks	Material is considered readily biodegradable under the conditions of this test.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.

Remarks for Data Reliability	Code 1. Guideline study.
References	Springborn Laboratories (2001) Ready Biodegradability by the closed bottle method. Study No. 1852.6173.
CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	The model predictions for 2-, 6-, or 8-pentadecanone are similar.
Method	Calculated
Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks to months and weeks, respectively.
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for Substance	
Method	Calculated
Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks to months and weeks, respectively.
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.

CAS	67662-98-0
Substance Name	3-Methyl-5-propylcyclohexanone
Remarks for Substance	
Method	Calculated

Test Type	
GLP	
Year	
Contact time (units)	
Innoculum	
Remarks for Test Conditions	
Degradation % after time	
Results	MITI Nonlinear Biodegradation Probability Model predicts that the substance is readily biodegradable. The Survey Model predicts ultimate and primary biodegradability within weeks to months and weeks, respectively.
Kinetic	
Time required for 10% degradation	
10 day window criteria	
Total degradation	
Classification	
Breakdown products (transient or stable)	
Remarks fields for results	
Conclusion remarks	The substance is concluded to be readily biodegradable.
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	BIOWIN EPI Suite (2000) US Environmental Protection Agency.

2.3 Fugacity

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data for 2-, 3-, 4-, and 5-nonanone are shown.

Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 19.3 to 24 hrs for all isomeric nonanones Water = 360 hrs for all isomeric nonanones Soil = 360 hrs for all isomeric nonanones Sediment = 1.44 x 10(+3) hrs for all isomeric nonanones
Estimated Distribution and Media Concentration	Air = 4.31% for 2-, 5.08% for 3-, 4.21% for 4-, and 5.675% for 5-nonanone Water = 30.5% for 2-, 32.7% for 3-, 32.0 for 4-, and 36.3% for 5-nonanone Soil = 64.8% for 2-, 62.0% for 3-, 63.5% for 4-, and 57.8% for 5-nonanone Sediment = 0.407% for 2-, 0.23
Remarks	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.

CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Data for 2-, 3-, 4-, and 5-decanone are shown.
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 17.4 to 21.3 hrs for all isomeric decanones Water = 360 hrs for all isomeric decanones Soil = 360 hrs for all isomeric decanones Sediment = 1.44 x 10(+3) hrs for all isomeric decanones
Estimated Distribution and Media Concentration	Air = 3.90% for 2-, 4.42% for 3-, 3.94% for 4-, and 5.38% for 5-decanone Water = 28.8% for 2-, 29.9% for 3-, 30.1% for 4-, and 34.9% for 5-decanone Soil = 66.2% for 2-, 65.2% for 3-, 65.6% for 4-, and 59.4% for 5-decanone Sediment = 1.09% for 2-, 0.44
Remarks	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the

	EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Data for 2-, 3-, 4-, 5-, and 6-undecanone are shown
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 15.9 to 19.3 hrs for all isomeric undecanones Water = 208-360 hrs for all isomeric undecanones Soil = 208-360 hrs for all isomeric undecanones Sediment = 832-1440 hrs for all isomeric undecanones
Estimated Distribution and Media Concentration	Air = 2.81% for 2-, 4.00% for 3-, 3.15% for 4-, 4.48% for 5- and 6-undecanone Water = 33.9% for 2-, 28.2% for 3-, 30.9% for 4-, and 35.9% for 5- and 6-undecanone Soil = 60.6% for 2-, 66.8% for 3-, 64.9% for 4-, and 58.9% for 5- and 6-undecanone Sediment
Remarks	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a

	five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Data for 2-, 3-, 4-, 5-, and 6-dodecanone are shown
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 14.6 to 17.2 hrs for all isomeric dodecanones Water = 208-360 hrs for all isomeric dodecanones Soil = 208-360 hrs for all isomeric dodecanones Sediment = 832-1440 hrs for all isomeric dodecanones
Estimated Distribution and Media Concentration	Air = 3.60% for 2-, 3.65% for 3-, 3.31% for 4-, 4.68% for 5-dodecanone Water = 26.7% for 2-, 26.7% for 3-, 26.8% for 4-, and 32.5% for 5-dodecanone Soil = 67.1% for 2-, 67.1% for 3-, 76.3% for 4-, and 61.0% for 5-dodecanone Sediment = 2.54% for 2-, 2.
Remarks	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.

References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data for 2,3-, 3,3-, 2,4-, and 2,6-dimethylcyclohexanones are shown
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 13.8 to 32.3 hrs for all isomeric dimethylcyclohexanones Water = 360-900 hrs for all isomeric dimethylcyclohexanones Soil = 360-900 hrs for all isomeric dimethylcyclohexanones Sediment = 1440-3600 hrs for all isomeric dime
Estimated Distribution and Media Concentration	Air = 2.62% for 3,3-, 2.59% for 2,3-, 3.02% for 2,4-, 3.24% for 2,6-dimethylcyclohexanones Water = 37.9% for 3,3-, 42.3% for 2,3-, 42.1% for 2,4-, 41.8% for 2,6-dimethylcyclohexanones Soil = 59.3% for 3,3-, 55.0% for 2,3-, 54.7% for 2,4-, 54.9% for 2,6-
Remarks	
Conclusion remarks	

Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 28.6 hr Water = 360 hr Soil = 360 hr Sediment = 1440 hr
Estimated Distribution and Media Concentration	Air = 6.6% Water = 38.15% Soil = 55.2% Sediment = 0.133%
Remarks	

Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.
CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	Data for 2-, 6-, and 8-pentadecanone
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 13.2 hr Water = 360 hr Soil = 360 hr Sediment = 1440 hr
Estimated Distribution and Media Concentration	Air = 1.93% Water = 16.3% Soil = 48.1% Sediment = 33.7%

Remarks	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.
CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for Substance	
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 17.7 hr Water = 360 hr Soil = 360 hr Sediment = 1440 hr
Estimated Distribution and Media Concentration	Air = 3.91% Water = 28.1% Soil = 67.1%

	Sediment = 0.86%
Remarks	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.
CAS	67662-98-0
Substance Name	3-Methyl-5-propylcyclohexanone
Remarks for Substance	
Model Conditions	
Test Type	Environmental Equilibrium Partitioning Model
Method	Mackay
Model Used (title, version, date)	Level III Fugacity-based Environmental Equilibrium Partitioning Model
Input parameters	MW, calculated VP, calculated MP, calculated Kow
Year	2000
Remarks for Test Conditions	
Media	
absorption coefficient	
Desorption	
Volatility	
Model data and results	Half-lives, t(1/2): Air = 9.58 hr Water = 360 hr Soil = 360 hr Sediment = 1440 hr

Estimated Distribution and Media Concentration	Air = 1.77% Water = 35.9% Soil = 62.0% Sediment = 6.353%
Remarks	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	Mackay D. (1991) Multimedia Environmental Models; The Fugacity Approach, Lewis Publishers, CRC Press, pp 67-183. Mackay D., A.DiGuardo, S.Paterson, G.Kicsi and C.E.Cowan (1996a) Assessing the fate of new and existing chemicals: a five stage process. Environmental Toxicology and Chemistry, 15(9), 1618-1626. Mackay D., A.DiGuardo, S.Paterson and C.E.Cowan (1996b) Evaluating the fate of a variety of types of chemicals using the EQC model. Environmental Toxicology and Chemistry, 15(9), 1627-1637.

3 ECOTOXICITY

3.1 Acute Toxicity to Fish

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Assay: 99+%
Method/guideline	96-hr LC50
Test Type	Flow-through
GLP	Yes
Year	1980
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Fathead minnows, 31 days of age and of mean length 21.0 mm, were treated with nominal concentrations of 0, 7.67, 11.8, 18.1, 27.8, or 42.8 mg/L of 2-nonanone in a flow through system at 25 C. The loading rate per tank was 2.76 g/L. Fish were maintained on 16 hours of light and 8 hours of darkness during the test. Fish were not fed 24 hours prior to and during the test. Tank concentrations of the test agent were monitored daily by GLC. Water quality was monitored for dissolved oxygen (6.6 mg/L), hardness (46.6 mg/L CaCO3), alkalinity (45.9 mg/L CaCO3), pH (7.60), and temperature (25.2 C). Experiments at each concentration were performed in duplicate. LC50 and EC50 values were calculated using corrected average tank concentrations and the Trimmed Spearman-Karber method.
Observations on precipitation	
Nominal concentrations as mg/L	0, 7.67, 11.8, 18.1, 27.8, or 42.8 mg/L
Measured concentrations as mg/L	1, 4.23, 7.77, 12.2, 20.4, or 29.9 mg/L
Unit	mg/L
Endpoint value	96-hr LC50 = 15.2 mg/L and. EC50=15.2 mg/L.
Reference substances (if used)	

Remarks fields for results	Affected fish lost schooling behavior, swam near tank bottom, and were hypoactive. Fish were darkly colored, had increased respiration, and lost equilibrium prior to death. Mortalities at 96 hrs: 27.8 mg/L 20/20; 42.8 mg/L, 20/20. No mortalities at lower concentrations.
Conclusion remarks	The LC50 of 2-nonanone in fathead minnows in a flow-through system is reported to be 15.2mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Geiger D.L., Poirer S.H., Brooke L. T. and Call D.J., eds (1986) Acute toxicities of organic chemicals to fathead minnows (Pimephales Promelas). Vol. III. Superior, Wisconsin: University of Wisconsin-Superior. Unpublished Report.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, and 5-nonanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 22.68 mg/L
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	

Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	502-56-7
Substance Name	5-Nonanone
Remarks for Substance	
Method/guideline	96-hr LC50
Test Type	
GLP	No
Year	1983
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Groups of twenty to twenty-five 30 day old fish were maintained at five different concentrations in flow-through systems for 96 hours in Lake Superior water. Deaths were recorded at 1, 3, 6, 12, 24, 48,72, and 96 hours. Concentrations of test substance were measured daily by CG analysis. Water analyses: 24-26 C, hardness = 45.5 mg/L CaCO3, alkalinity = 42.2 mg/L CaCO3, dissolved oxygen maintained at greater than 60% of saturation, pH= 7.5, 20-25 fish per dose, age= 30 day, weight = approximately 0.12 g.
Observations on precipitation	
Nominal concentrations as mg/L	Not given
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 31 mg/L
Reference substances (if used)	
Remarks fields for results	Substance was one of a series of 12 aliphatic ketones tested for acute toxicity in fathead minnows.
Conclusion remarks	The acute 96-hour LC50 of 5-nonanone is 31 mg/L at 25+/-1C.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.

Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Veith, G., Call, D., Brooke, L. (1983) Structure -Toxicity Relationships for Fathead Minnow (Pimephales promelas) Narcotic industrial chemicals. Canadian Journal of Fish. Aqua. Sci., 40, 743-748.
CAS	502-56-7
Substance Name	5-Nonanone
Remarks for Substance	Assay: 98%
Method/guideline	96-hr LC50
Test Type	Flow-through
GLP	Yes
Year	1980
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Fathead minnows, 30 days of age and of mean length 19.5 mm, were treated with nominal concentrations of 0, 13.5, 22.5, 37.6, or 62.6 mg/L of 5-nonanone in a flow through system at 25 C. The loading rate per tank was 0.464 g/L. Fish were maintained on 16 hours of light and 8 hours of darkness during the test. Fish were not fed 24 hours prior to and during the test. Tank concentrations of the test agent were monitored daily by GLC. Water quality was monitored for dissolved oxygen (7.0 mg/L), hardness (44.5 mg/L CaCO3), alkalinity (43.2 mg/L CaCO3), pH (7.75), and temperature (25.2 C). Experiments at each concentration were performed in duplicate. LC50 and EC50 values were calculated using corrected average tank concentrations and the Trimmed Spearman-Karber method.
Observations on precipitation	
Nominal concentrations as mg/L	0, 13.5, 22.5, 37.6, or 62.6 mg/L
Measured concentrations as mg/L	1, 5.2, 9.7, 16.1, 28, or 40.6 mg/L
Unit	mg/L
Endpoint value	96-hr LC50 = 31 mg/L(95% CI, 29.4-32.6 mg/L). EC50=31.0 mg/L (95% CI, 29.4-32.6 mg/L).
Reference substances (if used)	
Remarks fields for results	Affected fish became hypoactive, lost the schooling ability and equilibrium prior to death. Mortalities at 96 hrs: 37.6 mg/L 4/25

	and 5/25; 62.6mg/L, 25/25 and 25/25. No mortalities at lower concentrations.
Conclusion remarks	The LC50 of 5-nonanone in fathead minnows in a flow-through system is reported to be 31.0 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Geiger D.L., Poirer S.H., Brooke L. T. and Call D.J., eds (1986) Acute toxicities of organic chemicals to fathead minnows (Pimephales Promelas). Vol. III. Superior, Wisconsin: University of Wisconsin-Superior. Unpublished Report.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	
Method/guideline	96-hr LC50
Test Type	
GLP	No
Year	1983
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Groups of twenty to twenty-five 30 day old fish were maintained at five different concentrations in flow-through systems for 96 hours in Lake Superior water. Deaths were recorded at 1, 3, 6, 12, 24,48, 72, and 96 hours. Concentrations of test substance were measured daily by CG analysis. Water analyses: 24-26 C, hardness = 45.5 mg/L CaCO3, alkalinity = 42.2 mg/L CaCO3, dissolved oxygen maintained at greater than 60% of saturation, pH= 7.5, 20-25 fish per dose, age= 30 day, weight = approximately 0.12 g.
Observations on precipitation	
Nominal concentrations as mg/L	Not given
Measured concentrations as mg/L	
Unit	
Endpoint value	Acute 96-hr LC50 = 5.7 mg/L
Reference substances (if	

used)	
Remarks fields for results	Substance was one of a series of 12 aliphatic ketones tested for acute toxicity in fathead minnows.
Conclusion remarks	The acute 96-hour LC50 of 2-decanone is 5.7 mg/L at 25+/-1C.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Veith, G., Call, D., Brooke, L. (1983) Structure -Toxicity Relationships for Fathead Minnow (Pimephales promelas) Narcotic industrial chemicals. Canadian Journal of Fish. Aqua. Sci., 40, 743-748.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Assay: 95%
Method/guideline	96-hr LC50
Test Type	Flow-through
GLP	Yes
Year	1980
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Fathead minnows, 29 days of age and of mean length 18 mm, were treated with nominal concentrations of 0, 1.7, 2.9, 4.8, 7.9, or 13.2 mg/L of 2-decanone in a flow through system at 25 C. The loading rate per tank was 0.341 g/L. Fish were maintained on 16 hours of light and 8 hours of darkness during the test. Fish were not fed 24 hours prior to and during the test. Tank concentrations of the test agent were monitored daily by GLC. Water quality was monitored for dissolved oxygen (7.4 mg/L), hardness (41.7 mg/L CaCO3), alkalinity (43.0 mg/L CaCO3), pH (7.45), and temperature (24.7 C). Experiments at each concentration were performed in duplicate. LC50 and EC50 values were calculated using corrected average tank concentrations and the Trimmed Spearman-Karber method.
Observations on precipitation	
Nominal concentrations as mg/L	0, 1.7, 2.9, 4.8, 7.9, or 13.2 mg/L
Measured concentrations as mg/L	0, 0.5, 1.2, 2.4, 3.8, or 8.5 mg/L

Unit	mg/L
Endpoint value	96-hr LC50 = 5.7 mg/L(95% CI, 5.4-6.0 mg/L). EC50=5.7 mg/L (95% CI, 5.4-6.0 mg/L).
Reference substances (if used)	
Remarks fields for results	Affected fish became hypoactive, lost the schooling ability and equilibrium prior to death. Mortalities at 96 hrs: 7.9 mg/L 3/25 and 1/25; 13.2 mg/L, 25/25 and 25/25. No mortalities at lower concentrations.
Conclusion remarks	The LC50 of 2-decanone in fathead minnows in a flow-through system is reported to be 5.7 mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Geiger D.L., Poirer S.H., Brooke L. T. and Call D.J., eds (1986) Acute toxicities of organic chemicals to fathead minnows (Pimephales Promelas). Vol. III. Superior, Wisconsin: University of Wisconsin-Superior. Unpublished Report.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, and 5-decanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 8.627 mg/L

Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Assay: 95%
Method/guideline	96-hr LC50
Test Type	Flow-through
GLP	Yes
Year	1980
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Fathead minnows, 31 days of age and of mean length 21.9 mm, were treated with nominal concentrations of 0, 1.07, 1.64, 2.52, 3.87, or 5.95 mg/L of 2-undecanone in a flow through system at 25 C. The loading rate per tank was 3.14 g/L. Fish were maintained on 16 hours of light and 8 hours of darkness during the test. Fish were not fed 24 hours prior to and during the test. Tank concentrations of the test agent were monitored daily by GLC. Water quality was monitored for dissolved oxygen (6.6 mg/L), hardness (48.8 mg/L CaCO3), alkalinity (45.4 mg/L CaCO3), pH (7.67), and temperature (25.1 C). Experiments at each concentration were performed in duplicate. LC50 and EC50 values were calculated using corrected average tank concentrations and the Trimmed Spearman-Karber method.
Observations on precipitation	
Nominal concentrations as mg/L	0, 1.07, 1.64, 2.52, 3.87, or 5.95 mg/L
Measured concentrations as mg/L	0.16, 0.42, 0.61, 1.04, 1.87, or 3.24 mg/L
Unit	mg/L

Endpoint value	96-hr LC50 = 1.50 mg/L (95% CI, 1.39-1.62 mg/L) and. EC50=1.50 mg/L (95% CI, 1.39-1.62 mg/L)
Reference substances (if used)	
Remarks fields for results	Affected fish lost schooling behavior, swam near tank bottom, and were hypoactive. Fish were darkly colored, had increased respiration, and lost equilibrium prior to death. Mortalities at 96 hrs: 3.87 mg/L 18/20; 5.95 mg/L, 20/20. No mortalities at lower concentrations.
Conclusion remarks	The LC50 of 2-undecanone in fathead minnows in a flow-through system is reported to be 1.50mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Geiger D.L., Poirer S.H., Brooke L. T. and Call D.J., eds (1986) Acute toxicities of organic chemicals to fathead minnows (Pimephales Promelas). Vol. III. Superior, Wisconsin: University of Wisconsin-Superior. Unpublished Report.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, 5-, and 6-undecanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 3.255 mg/L

Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Assay: 99%
Method/guideline	96-hr LC50
Test Type	Flow-through
GLP	Yes
Year	1980
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Fathead minnows, 33 days of age and of mean length 18.3 mm, were treated with nominal concentrations of 0, 0.90, 1.38, 2.12, 3.26, or 5.01 mg/L of 2-dodecanone in a flow through system at 24.8C. The loading rate per tank was 1.76 g/L. Fish were maintained on 16 hours of light and 8 hours of darkness during the test. Fish were not fed 24 hours prior to and during the test. Tank concentrations of the test agent were monitored daily by GLC. Water quality was monitored for dissolved oxygen (6.8 mg/L), hardness (44.4 mg/L CaCO3), alkalinity (44.6 mg/L CaCO3), pH (7.6), and temperature (24.8 C). Experiments at each concentration were performed in duplicate. LC50 and EC50 values were calculated using corrected average tank concentrations and the Trimmed Spearman-Karber method.
Observations on precipitation	
Nominal concentrations as mg/L	0, 0.90, 1.38, 2.12, 3.26, or 5.01 mg/L
Measured concentrations as mg/L	0.10, 0.36, 0.59, 0.71, 1.14, or 2.61 mg/L
Unit	mg/L

Endpoint value	96-hr LC50 = 1.18 mg/L (95% CI, 1.02-1.37 mg/L) and. EC50=1.18 mg/L (95% CI, 1.02-1.37 mg/L)
Reference substances (if used)	
Remarks fields for results	Affected fish lost schooling behavior, swam near tank bottom, and were hypoactive. Fish were darkly colored, had increased respiration, and lost equilibrium prior to death. Mortalities at 96 hrs: 2.12 mg/L 1/20; 3.26 mg/L, 9/20; 5.01 mg/L 20/20. No mortalities at lower concentrations.
Conclusion remarks	The LC50 of 2-dodecanone in fathead minnows in a flow-through system is reported to be 1.18mg/L
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Geiger D.L., Poirer S.H., Brooke L. T. and Call D.J., eds (1986) Acute toxicities of organic chemicals to fathead minnows (Pimephales Promelas). Vol. III. Superior, Wisconsin: University of Wisconsin-Superior. Unpublished Report.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, 5-, and 6-dodecanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 1.200 mg/L

Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for Substance	Calculated data for 2,3-, 2,4-, or 2,6-dimethylcyclohexanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 102.014 mg/L
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.

References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related ketone, 3-5,5-trimethyl-2-cyclhexenone.
Method/guideline	96-hr LC50
Test Type	Static
GLP	No
Year	1981
Species/Strain/Supplier	Fish/Bluegill
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Groups of 10, 30 day old fish were maintained at five different concentrations in flow-through systems for 96 hours in Lake Superior water. Deaths were recorded at 1, 3, 6, 12, 24, 48, 72, and 96 hours. Concentrations of test substance were measured daily by CG analysis. Water analyses: 24-26 C, hardness = 45.5 mg/L CaCO3, alkalinity = 42.2 mg/L, pH = 7.9 to 6.5, temperature 21-23C. Carrier solvent used 1,6-hexanediol, acetone, or dimethylformamide. LC50's were calculated by the log probit method (Litchfield and Wilcoxon, 1949).
Observations on precipitation	Test chemical formed slick on water surface.
Nominal concentrations as mg/L	Not given
Measured concentrations as mg/L	
Unit	
Endpoint value	LC50 = 220 mg/L (95% CI, 180-250 mg/L)
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	The acute 96-hr LC50 of isophorone in bluegills is estimated to be 220 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Buccafusco R.J., Ells S.J., and LeBlanc G. A. (1981) Acute toxicity of priority pollutants to Bluegill. Bulletin of Environmental

	Contaminant Toxicology, 26, 446-452.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 93.554 mg/L
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for dehydro analog, 6-methyl-5-hepten-2-one.

Method/guideline	96-hr LC50
Test Type	Flow-through
GLP	No
Year	1983
Species/Strain/Supplier	Minnows/Fathead/Environmental Research Laboratories/Duluth
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Groups of twenty to twenty-five 30 day old fish were maintained at five different concentrations in flow-through systems for 96 hours in Lake Superior water. Deaths were recorded at 1, 3, 6, 12, 24, 48, 72, and 96 hours. Concentrations of test substance were measured daily by CG analysis. Water analyses: 24-26 C, hardness = 45.5 mg/L CaCO3, alkalinity = 42.2 mg/L CaCO3, dissolved oxygen maintained at greater than 60% of saturation, pH = 7.5, 20-25 fish per dose, age = 30 day, weight = approximately 0.12 g.
Observations on precipitation	
Nominal concentrations as mg/L	Not given
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 85.7 mg/L
Reference substances (if used)	
Remarks fields for results	Substance was one of a series of 12 aliphatic ketones tested for acute toxicity in fathead minnows.
Conclusion remarks	The acute 96-hour LC50 of 6-methyl-5-hepten-2-one is 85.7 mg/L at 25+/-1C.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Veith, G., Call, D., Brooke, L. (1983) Structure -Toxicity Relationships for Fathead Minnow (Pimephales promelas) Narcotic industrial chemicals. Canadian Journal of Fish. Aqua. Sci., 40, 743-748.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for isomer, 2-octanone.

Method/guideline	96-hr LC50
Test Type	Flow-through
GLP	Yes
Year	1985
Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Juvenile fathead minnows, 28-34 days of age, were treated with five concentrations of 2-octanone in a flow through system at 25 C. Fish were maintained on 16 hours of light and 8 hours of darkness during the test. Fish were not fed 24 hours prior to and during the test. Tank concentrations of the test agent were monitored daily by GLC. Water quality was monitored for dissolved oxygen (>80% saturation), alkalinity (44.6 mg/L CaCO3), pH (7.6), and temperature (25+/-0.5C). Experiments at each concentration were performed in duplicate. LC50 and EC50 values were calculated using corrected average tank concentrations and the Trimmed Spearman-Karber method.
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	Acute 96-hr LC50 = 63 mg/L (95% CI, 60.9-65.2 mg/L)
Reference substances (if used)	
Remarks fields for results	Multiple acute test were run for 2-octanone.
Conclusion remarks	The acute 96-hr LC50 of 2-octanone in fathead minnows is 63 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Broderius S. and Kahl M. (1985) Acute toxicity of organic chemical mixtures to the fathead minnow. Aquatic Toxicology, 6, 307-322.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone

Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 68.698 mg/L
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for isomer, 2-octanone.
Method/guideline	96-hr LC50
Test Type	
GLP	No
Year	1983

Species/Strain/Supplier	Minnows/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Groups of twenty to twenty-five 30 day old fish were maintained at five different concentrations in flow-through systems for 96 hours in Lake Superior water. Deaths were recorded at 1, 3, 6, 12, 24, 48, 72, and 96 hours. Concentrations of test substance were measured daily by CG analysis. Water analyses: 24-26 C, hardness = 45.5 mg/L CaCO3, alkalinity = 42.2 mg/L CaCO3, dissolved oxygen maintained at greater than 60% of saturation, pH = 7.5, 20-25 fish per dose, age= 30 day, weight = approximately 0.12 g.
Observations on precipitation	
Nominal concentrations as mg/L	Not given
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 36 mg/L
Reference substances (if used)	
Remarks fields for results	Substance was one of a series of 12 aliphatic ketones tested for acute toxicity in fathead minnows
Conclusion remarks	The acute 96-hour LC50 of 2-octanone is 36 mg/L at 25+/-1C.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Veith, G., Call, D., Brooke, L. (1983) Structure -Toxicity Relationships for Fathead Minnow (Pimephales promelas) Narcotic industrial chemicals. Canadian Journal of Fish. Aqua. Sci., 40, 743-748.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for structurally related substance 2-hexanone,5-methyl-.
Method/guideline	
Test Type	Static
GLP	No
Year	1978

Species/Strain/Supplier	Minnow/Fathead
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	Water was filter-treated lake water with residual chlorine chemically removed. 10 fish/concentration levels were used. Exposure solutions were submitted for temperature, dissolved oxygen, and pH concentration determinations at 0, 24, 48, 72 and 96 hours. Observations for stress and mortality were conducted at 0, 6, 24, 48, 72 and 96 hours.
Observations on precipitation	
Nominal concentrations as mg/L	100 ul/L
Measured concentrations as mg/L	
Unit	
Endpoint value	LC50 greater than 100 ul/L; NOEC > 100 ul/L
Reference substances (if used)	
Remarks fields for results	Exposure temperature was 19 deg C, pH ranged from 7.4 to 7.9, and dissolved oxygen ranged from 4.8 to 8.7 mg/L.
Conclusion remarks	The acute 96-hr LC50 =100 ul/L LC50 value indicates that the test substance would not be classified according to the European Union's labelling directive and would correspond to a "low concern level" according to the US EPA's assessment criteria.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Eastman Kodak Co. (1978) An acute aquatic effects test with the Fathead Minnow (Pimephales promelas);Environmental Sciences Section, Health and Environment Laboratories, HAEL No. 78-0260.
CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	

Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 3.788 mg/L
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	67662-98-0
Substance Name	3-Methyl-5-propylcyclohexanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	

Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	96-hr LC50 = 14.95 mg/L
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Species/Strain/Supplier	
Analytical monitoring	
Exposure period (unit)	96 hour
Remarks for Test Conditions	
Observations on precipitation	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	

Endpoint value	96-hr LC50 = 0.061 mg/L
Reference substances (if used)	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	123-18-2
Substance Name	2,6,8-Trimethyl-4-nonanone (IBHK)
Remarks for Substance	Assay: 91+%
Method/guideline	OECD Guideline No. 203, Fish Acute Toxicity Test. Directive 92/69/EEC, C.1 Acute Toxicity to Fish. EPA OTS 797.1440, Fish Acute Toxicity Test.
Test Type	Static
GLP	Yes
Year	2003
Species/Strain/Supplier	Oncorhynchus mykiss (Fish, fresh water
Analytical monitoring	GC Analysis
Exposure period (unit)	96 hour
Remarks for Test Conditions	This study evaluated the acute toxicity of the test substance to rainbow trout (Oncorhynchus mykiss) over a 96-hour exposure period under static conditions. A preliminary study found no mortality at nominal concentrations of 0, 5, 10, 50 and 100 mg IBHK/L after 96 hr. Sublethal effects such as lethargy and partial loss of equilibrium were observed at the 50 and 100 mg/L dose levels, however, these effects may have been due to the presence of insoluble test material in the solutions. Test solutions for the definitive study were prepared in duplicate at nominal concentrations of 6.25, 12.5, 25.0, 50.0 and 100 mg IBHK/L. All concentrations were corrected for the 91.3% purity. Duplicate negative control solutions (dilution water) were maintained concurrently. Dilution water was Lake Huron water supplied to the laboratory by the City of Midland Water Treatment Plant, subsequently sand-filtered, pH-adjusted with gaseous CO2, carbon-filtered and UV-irradiated, and monitored regularly. The dilution water used in this study was characterized as follows: hardness of 66-90 mg/L as CaCO3, alkalinity of 40-48 mg/L as CaCO3, pH of 7.3, conductivity of 151-171 mmhos/cm and chlonne <10 ppb. Test vessels were 12-1 glass beakers which were filled with 101 of test solution. Ten fish were impartially introduced to each replicate test vessel at test initiation. Loading did not exceed 1.0-g fish per liter of test solution. Fish were not fed during the study. Terminal body weight and standard length were recorded for all surviving fish at test termination. Fish were

	observed dally for mortality and sublethal effects. Mortality was defined as a lack of response to prodding of the caudal peduncle accompanied by an absence of opercular movement. Dissolved oxygen (DO), pH and temperature were recorded at test initiation and daily thereafter. Over the course of the study, DO levels averaged 8.3 +/- 0.7, averaged 85% of saturation and remained greater than or equal to 72% over the g6-hour exposure period. The pH averaged 7.5 +/- 0.2 over the course of the study. Temperature in the test vessels averaged 15.2 ± 0.5 deg C.
Observations on precipitation	
Nominal concentrations as mg/L	1.24 mg/L (tested at solubility limit)
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	LC50 (48-hr) > 1.24 mg/L; LC50 (72-hr) > 1.24 mg/L; LC50 (96-hr) > 1.24 mg/L; NOEC (96-hr) = 1.24 mg/L
Reference substances (if used)	
Remarks fields for results	No fish mortality or sublethal effects were observed at or below the highest measured concentration tested of 1.24 mg/L or in the water control during the conduct of this study. The temperature, pH and dissolved oxygen concentration during this study were maintained at 15.2 ± 0.5°C, 7.5 ± 0.2 and 8.3 ± 0.7 mg/l (or >85% saturation), respectively. Pooled standard length and weight means (+ sd) for all surviving fish (treatments and controls) were 4.4 ± 0.3 cm and 636 ± 127 rag, respectively.
Conclusion remarks	LC50=1.24 mg/L represents the maximum solubility of IBHK in this test medium using the test solution preparation procedure employed
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Dow Chemical (2003) Acute toxicity of 2,6,8-trimethyl-4-nonanone in fish. Unpublished Report.

3.2 Acute Toxicity to Aquatic Invertebrates

CAS	821-55-6
Substance Name	2-Nonanone

Remarks for Substance	Calculated data for 2-, 3-, 4-, or 5-nonanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr EC50 = 26.52 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	925-78-0
Substance Name	3-Nonanone
Remarks for Substance	Data are for homologue, 3-octanone.
Method/guideline	Experimental
Test Type	24-hour LC50 static test
GLP	No

Year	1977
Analytical procedures	
Species/Strain	Daphnia magna
Test details	24 hours
Remarks for Test Conditions	Daphnia magna (30/group, 24 hours old) were maintained in chlorine free tap water saturated with oxygen, pH of 7.7-7.7 and temperature of 20-22 °C. The LC50, LC0 and LC100 were determined.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
EC50, EL50, LC0, at 24,48 hours	24 hour LC50 = 517, LC0 = 175 mg/mL
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	The study was reported in German with an English summary, but the results are considered reliable.
References	Bringmann G. and Kuehn, R. (1977) Befunde der Schadwirkung wassergefaehrdender Stoffe gegen Daphnia magna. [Results of the damaging effects of water pollutants on Daphnia magna.] A Wasser Abwasser Forsch., 10(5), :161-166.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, or 5-decanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	

Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr EC50 = 10.04 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, 5- or 6-undecanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	

Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr EC50 = 3.92 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, 5- or 6-dodecanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L

EC50, EL50, LC0, at 24,48 hours	96-hr EC50 = 1.52 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr EC50 = 93.55 at 25 °C
Biological observations	
Control response satisfactory	

Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for Substance	Calculated data for 2,3-, 2,4-, or 2,6-dimethylcyclohexanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr EC50 = 109.0 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	

Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for Substance	Data are for homologue, 2-methylcyclohexanone.
Method/guideline	Experimental
Test Type	24-hour LC50 static test
GLP	No
Year	1977
Analytical procedures	
Species/Strain	Daphnia magna
Test details	24 hours
Remarks for Test Conditions	Daphnia magna (30/group, 24 hours old) were maintained in chlorine free tap water saturated with oxygen, pH of 7.7-7.7 and temperature of 20-22 C. The LC50, LC0 and LC100 were determined.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
EC50, EL50, LC0, at 24,48 hours	24 hour LC50 = 435, LC0 = 125, LC100 = 1000 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.

Remarks for Data Reliability	The study was reported in German with an English summary, but the results are considered reliable.
References	Bringmann G. and Kuehn, R. (1977) Befunde der Schadwirkung wassergefaehrdender Stoffe gegen Daphnia magna. [Results of the damaging effects of water pollutants on Daphnia magna.] A Wasser Abwasser Forsch., 10(5), 161-166.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr EC50 = 74.38 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for structurally related substance 5-methyl-2-hexanone.
Method/guideline	
Test Type	Acute immobilization, Static
GLP	No
Year	1978
Analytical procedures	Yes, exposure solutions, temp., pH, dissolved oxygen
Species/Strain	Daphnid/daphnia magna
Test details	96 hour
Remarks for Test Conditions	Water was filter-treated lake water with residual chlorine chemically removed. 10 Daphnids per dose level were used. Exposure solutions were submitted for temperature, dissolved oxygen, and pH concentration determinations at 0, 24, 48, 72, and 96-hours. Observations for stress and mobility were conducted at 0, 6, 24, 48, 72 and 96 hours.
Nominal concentrations as mg/L	100 ul/L
Measured concentrations as mg/L	
Unit	
EC50, EL50, LC0, at 24,48 hours	EC50 96-hour greater than 100 ul/L; NOEC greater than 100 ul/L.
Biological observations	The Daphnia exhibited behaviour comparable to controls at all test concentrations.
Control response satisfactory	
Appropriate statistical evaluations	NA; no effects were noted at this concentration.
Remarks fields for results	Exposure temperature remained at 19 °C throughout the test, pH was 7.4-7.9, and dissolved oxygen was 4.8-8.7 mg/L.
Conclusion remarks	The LC50 value indicated that the test substance would not be classified according to the European Union's labelling directive and would correspond to a "low concern level" according to the US EPA's assessment criteria.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.

References	Eastman Kodak Co. (2000) An acute aquatic effects test with the Daphnid (*daphnia magna*); Environmental Sciences Section, Health and Environment Laboratories, HAEL No. 78-0260.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for homologue, 5-methyl-2-hexanone.
Method/guideline	Experimental
Test Type	24-hour LC50 static test
GLP	No
Year	1977
Analytical procedures	
Species/Strain	Daphnia magna
Test details	24 hours
Remarks for Test Conditions	Daphnia magna (30/group, 24 hours old) were maintained in chlorine free tap water saturated with oxygen, pH of 7.7-7.7 and temperature of 20-22 °C. The LC50, LC0 and LC100 were determined.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
EC50, EL50, LC0, at 24,48 hours	24 hour LC50 = 170, LC0 = 910, LC100 = 2000 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	The study was reported in German with an English summary, but the results are considered reliable.
References	Bringmann G. and Kuehn, R. (1977) Befunde der Schadwirkung wassergefaehrdender Stoffe gegen Daphnia magna. [Results of the damaging effects of water pollutants on

	Daphnia magna.] A Wasser Abwasser Forsch., 10(5), 161-166.
CAS	5440-89-1
Substance Name	5-Ethyl-2-nonanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr LC50 = 4.54 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	2345-28-0
Substance Name	2-Pentadecanone

Remarks for Substance	Calculated data for 2-, 6-, or 8-pentadecanone are equivalent,
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr LC50 = 0.084 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	67662-98-0
Substance Name	3-Methyl-5-propylcyclohexanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	

Year	
Analytical procedures	
Species/Strain	Daphnia magna
Test details	96 hours
Remarks for Test Conditions	
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
EC50, EL50, LC0, at 24,48 hours	96-hr LC50 = 17.09 at 25 °C
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	123-18-2
Substance Name	2,6,8-Trimethyl-4-nonanone (IBHK)
Remarks for Substance	Assay: 91+%
Method/guideline	OECD Guideline No. 202, Daphnia sp., Acute immobilization Test, Part 1.Directive 92/69/EEC, C.2 Acute Toxicity for Daphnia. EPA OTS CFR 797.1300, Daphnid Acute Toxicity Test
Test Type	48-hour EC50 static test
GLP	Yes
Year	2003
Analytical procedures	No
Species/Strain	Daphnia magna

Test details	48 hours
Remarks for Test Conditions	This study evaluated the acute toxicity of the test substance to <24-hour old daphnia (Daphnia magna Straus) over a 48-hour exposure period under static-renewal conditions. A preliminary study of dose levels 25, 50 and 100 rng IBHK/L found 40 and 50% immobility/mortality at nominal concentrations of 50 and 100 mg IBHK/L, respectively at 24 hours of exposure. Following 48 hours of exposure, immobility increased to 90 and 100% at 50 and 100 mg IBHK/L, respectively. No immobility was observed in the water control. Based on these results, the 48-hour EC50 was estimated to be below the nominal concentration of 25 mg IBHK/L. Due to the results of this preliminary study, the test solutions for the definitive study were prepared in duplicate at nominal concentrations of 1.56, 3.13, 6.25, 12.5, 25.0, 50.0, and 100 mg IBHK/L. All concentrations were adjusted for the purity of 91.3%. Duplicate negative control solutions (dilution water) were maintained concurrently. Dilution water was Lake Huron water supplied to the laboratory by the City of Midland Water Treatment Plant, subsequently sand-filtered, pH-adjusted with gaseous CO2, carbon-filtered and UV-irradiated, adjusted to hardness of about 170 mg/L as CaCO3, then autoclaved at 250°F and 18 psi for 30 min. The dilution water used in this study was characterized as follows: hardness of 158-174 mg/L as CaCO3, alkalinity of 36-38 mg/L as CaCO3, pH of 7.6 $\pm$ 0.1, conductivity of 417-434 mmhos/cm and chlorine <10 ppb. Test vessels were 250-ml glass jars containing 200 ml of test solution. Ten daphnia were impartially introduced to each replicate test vessel at test initiation. Daphnia were observed every 24 hours for immobility, mortality and any other sublethal effects. Immobility was defined as the inability to swim within 15 seconds after gentle agitation of the test container. Dissolved oxygen, pH and temperature were recorded every 24 hours.
Nominal concentrations as mg/L	1.56, 3.13, 6.25, 12.5, 25.0, 50.0, and 100 mg IBHK/L
Measured concentrations as mg/L	
Unit	
EC50, EL50, LC0, at 24,48 hours	EC50 (48-hr) = 3.41 mg/L (95% confidence interval = 2.71-4.20 mg/L; Probit slope = 4.1 with 95% confidence interval of 2.8-5.4); and NOEC (48-hr) = 0.949 mg/L.
Biological observations	
Control response satisfactory	Yes
Appropriate statistical evaluations	Yes
Remarks fields for results	Immobilization was reported for 40% and 50% of the daphnia at the 11.6 and 9.19 mg/L dose levels at 24 hours. Following 48 hours, immobility was observed in 100%, 95%, 65% and 25% of the daphnia at the 11.6, 9.19, 4.51, and 2.12 mg/L, respectively. The light intensity, temperature, pH and dissolved oxygen concentration during this study were maintained at 1776 $\pm$ 34 lux, 20.0 $\pm$ 1°C, 7.6 ± 0.1 and 8.9 ± 0.1 mg/L (or >/= 97% saturation), respectively.
Conclusion remarks	24-hour EC50 could not be calculated using the U.S. EPA Probit or Trimmed Spearman-Karber statistical programs due to the insufficient biological response following 24 hours of exposure.

	EC50 (48-hr) = 3.41 mg/L (95% confidence interval = 2.71-4.20 mg/L; Probit slope = 4.1 with 95% confidence interval of 2.8-5.4); and NOEC (48-hr) = 0.949 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Dow Chemical (2003) Acute toxicity of 2,6,8-trimethyl-4-nonanone in *Daphnia magna*. Unpublished Report.

3.3 Acute Toxicity to Aquatic Plants

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data are for structurally related substance 2-heptanone, purity 99.8%.
Method/guideline	OECD: TG-201
Test Type	Growth inhibition of algae
GLP	Yes
Year	1998
Species/Strain/Supplier	Selenastrum capricornutum
Endpoint basis	Cell concentrations and growth rate
Exposure period (duration)	72 hours
Analytical monitoring	Temp., light intensity, rpm, test substance
Remarks for Test Conditions	
Nominal concentrations as mg/L	12.5, 25, 50, 100 and 200
Measured concentrations as mg/L	6.2, 11.9, 22.1, 42.7, 86.3 mg/L
Unit	
Endpoint value	0-72 hr - EbC50 was 75.5 mg/L; ErC50 was 98.2 mg/L
NOEC, LOEC or NOEL, LOEL	72 hour NOEC was estimated to be 42.7 mg/L

Biological observations	No deformed cells were noted.
Control response satisfactory	Yes
Appropriate statistical evaluations	
Remarks fields for results	A mean illumination of 741 +/- 1.7 foot-candles was maintained. The mean temperature was 24 °C and pH ranged from 7.3-7.7. Cultures were oscillated at 100 rpm. The significant loss (up to 82% over the course of the study) in the material was attributed to volatilization. No protocol deviations were noted.
Conclusion remarks	The 72-hour EbC50 and ErC50 values indicate that the test substance would be classified as "harmful to aquatic organisms" according to the European Union's labelling directive and would be classified in a "moderate concern level" according to US EPA's.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Eastman Kodak Co. (1998) A growth inhibition test with alga, Selenastrum capricornutum. Enviromental Sciences Section, Health and Environment Laboratories, Eastman Kodak Co., Rochester, NY.

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	
Method/guideline	TETRATOX Assay
Test Type	48 hr IGC50 test
GLP	No
Year	1997
Species/Strain/Supplier	Tetrahymena pyriformis/GL-C
Endpoint basis	
Exposure period (duration)	40 hour
Analytical monitoring	GC
Remarks for Test Conditions	A 40 hour static assay was conducted to measure the 50% growth inhibitory concentration of the test substance on Tetrahymena pyriformis. The test was allow to run through 8-9 cell cycles. Semidefined proteose-peptone-based medium were inoculated to a density of 2500 cells/ml with log-growth-phase ciliates in the presence of the test material in DMSO. The test material was evaluated in each of three replicates at 6-8 different concentrations. Controls were inoculated with T.

	pyriformis in the absence of test material. Following incubation at 27 C, the population density of T. pyriformis was measured at 540 nM. The 50% growth inhibitory concentration was determined from probit analysis of absorbance values and concentrations.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	40-hr IGC50 = 33.26 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	Yes, Probit Anaylsis (Finney, 1971)
Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 2-nonanone required for 50% growth inhibition of Tetrahymena pyriformis is 33.26 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. (1997) TETRATOX: Tetrahymena pyriformis population growth impairment endpoint-asurrogate for fish lethality. Toxicology Methods, 7, 289-309.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Assay greater than 95%, Data are for homolog, 2-octanone.
Method/guideline	Schultz, 1990
Test Type	48 hr EC50 test
GLP	No
Year	1990
Species/Strain/Supplier	Tetrahymena pyriformis
Endpoint basis	
Exposure period (duration)	48 hour

Analytical monitoring	GC
Remarks for Test Conditions	48 hour population densities of axanic cultures of tetrahymena pyriformis were measured spectraphotometrically at 540 nm. Each chemical was tested in duplicate for at least 3 replicates. Each replicate was a five step graded concentration series. The 50% growth inhibition concentration was determined for each chemical using Probit Analysis. ll concentrations were measured using GC Analysis using HP Model 5840A.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	48-hr EC50 = 224 mg/L
Biological observations	Abiotic loss of ketones was between 20-60% over the 48 hr period.
Control response satisfactory	
Appropriate statistical evaluations	Yes, Probit Anaylsis of SAS Institute, 1985.
Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 2-Octanone required for 50% growth inhibition of Tetrahymena pyriformis is 224 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. Wyatt N.L., Lin D.T. (1990) Structure-toxicity of nonpolar narcotics: A comparison of data from the Tetrahymen, Photobacterium and Pimephales systems
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, or 5-nonanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	2000

Species/Strain/Supplier	Green algae
Endpoint basis	
Exposure period (duration)	96 hours
Analytical monitoring	
Remarks for Test Conditions	Based on: log KOW = 4.80, water solubility = 90 mg/L
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	
NOEC, LOEC or NOEL, LOEL	96-hr EC50 =16.62 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data are for structurally related substance 2-heptanone.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	2000
Species/Strain/Supplier	Green algae
Endpoint basis	

Exposure period (duration)	96 hours
Analytical monitoring	
Remarks for Test Conditions	Based on: log KOW = 4.80, water solubility = 90 mg/L
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	
NOEC, LOEC or NOEL, LOEL	96-hr EC50 = 98.3 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.

CAS	4485-09-0
Substance Name	4-Nonanone
Remarks for Substance	Assay greater than 95%, Data are for homolog, 4-heptanone.
Method/guideline	Schultz, 1990
Test Type	48 hr EC50 test
GLP	No
Year	1990
Species/Strain/Supplier	Tetrahymena pyriformis
Endpoint basis	
Exposure period (duration)	48 hour
Analytical monitoring	GC

Remarks for Test Conditions	48 hour population densities of axanic cultures of tetrahymena pyriformis were measured spectraphotometrically at 540 nm. Each chemical was tested in duplicate for at least 3 replicates. Each replicate was a five step graded concentration series. The 50% growth inhibition concentration was determined for each chemical using Probit Analysis. All concentrations were measured using GC Analysis using HP Model 5840A.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	48-hr EC50 = 679 mg/L
Biological observations	Abiotic loss of ketones was between 20-60% over the 48 hr period.
Control response satisfactory	
Appropriate statistical evaluations	Yes, Probit Anaylsis of SAS Institute, 1985.
Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 4-Heptanone required for 50% growth inhibition of Tetrahymena pyriformis is 679 mg/L
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. Wyatt N.L., Lin D.T. (1990) Structure-toxicity of nonpolar narcotics: A comparison of data from the Tetrahymen, Photobacterium and Pimephales systems
CAS	502-56-7
Substance Name	5-Nonanone
Remarks for Substance	Assay greater than 95%
Method/guideline	Schultz, 1990
Test Type	48 hr EC50 test
GLP	No
Year	1990
Species/Strain/Supplier	Tetrahymena pyriformis

Endpoint basis	
Exposure period (duration)	48 hour
Analytical monitoring	GC
Remarks for Test Conditions	48 hour population densities of axanic cultures of tetrahymena pyriformis were measured spectraphotometrically at 540 nm. Each chemical was tested in duplicate for at least 3 replicates. Each replicate was a five step graded concentration series. The 50% growth inhibition concentration was determined for each chemical using Probit Analysis. All concentrations were measured using GC Analysis using HP Model 5840A.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	48-hr EC50 = 145 mg/L
Biological observations	Abiotic loss of ketones was between 20-60% over the 48 hr period.
Control response satisfactory	
Appropriate statistical evaluations	Yes, Probit Anaylsis of SAS Institute, 1985.
Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 5-Nonanone required for 50% growth inhibition of Tetrahymena pyriformis is 145 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. Wyatt N.L., Lin D.T. (1990) Structure-toxicity of nonpolar narcotics: A comparison of data from the Tetrahymen, Photobacterium and Pimephales systems.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	
Method/guideline	TETRATOX Assay
Test Type	48 hr IGC50 test

GLP	No
Year	1997
Species/Strain/Supplier	Tetrahymena pyriformis/GL-C
Endpoint basis	
Exposure period (duration)	40 hour
Analytical monitoring	GC
Remarks for Test Conditions	A 40 hour static assay was conducted to measure the 50% growth inhibitory concentration of the test substance on Tetrahymena pyriformis. The test was allowed to run through 8-9 cell cycles. Semidefined proteose-peptone-based medium were inoculated to a density of 2500 cells/ml with log-growth-phase ciliates in the presence of the test material in DMSO. The test material was evaluated in each of three replicates at 6-8 different concentrations. Controls were inoculated with T. pyriformis in the absence of test material. Following incubation at 27 C, the population density of T. pyriformis was measured at 540 nM. The 50% growth inhibitory concentration was determined from probit analysis of absorbance values and concentrations.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	40-hr IGC50 = 44.21 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	Yes, Probit Anaylsis (Finney, 1971)
Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 2-decanone required for 50% growth inhibition of Tetrahymena pyriformis is 44.21 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. (1997) TETRATOX: Tetrahymena pyriformis population growth impairment endpoint-asurrogate for fish lethality. Toxicology Methods, 7, 289-309.

CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Assay greater than 95%
Method/guideline	Schultz, 1990
Test Type	48 hr EC50 test
GLP	No
Year	1990
Species/Strain/Supplier	Tetrahymena pyriformis
Endpoint basis	
Exposure period (duration)	48 hour
Analytical monitoring	GC
Remarks for Test Conditions	48 hour population densities of axanic cultures of tetrahymena pyriformis were measured spectraphotometrically at 540 nm. Each chemical was tested in duplicate for at least 3 replicates. Each replicate was a five step graded concentration series. The 50% growth inhibition concentration was determined for each chemical using Probit Analysis. All concentrations were measured using GC Analysis using HP Model 5840A.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	48-hr EC50 = 49.3 mg/L
Biological observations	Abiotic loss of ketones was between 20-60% over the 48 hr period.
Control response satisfactory	
Appropriate statistical evaluations	Yes, Probit Analysis of SAS Institute, 1985.
Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 2-Decanone required for 50% growth inhibition of Tetrahymena pyriformis is 49.3 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.

Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. Wyatt N.L., Lin D.T. (1990) Structure-toxicity of nonpolar narcotics: A comparison of data from the Tetrahymen, Photobacterium and Pimephales systems.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, or 5-decanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	2000
Species/Strain/Supplier	Green algae
Endpoint basis	
Exposure period (duration)	96 hours
Analytical monitoring	
Remarks for Test Conditions	Based on: log KOW = 4.80, water solubility = 90 mg/L
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	
NOEC, LOEC or NOEL, LOEL	96-hr EC50 =6.728 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.

References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	
Method/guideline	TETRATOX Assay
Test Type	48 hr IGC50 test
GLP	No
Year	1997
Species/Strain/Supplier	Tetrahymena pyriformis/GL-C
Endpoint basis	
Exposure period (duration)	40 hour
Analytical monitoring	GC
Remarks for Test Conditions	A 40 hour static assay was conducted to measure the 50% growth inhibitory concentration of the test substance on Tetrahymena pyriformis. The test was allowed to run through 8-9 cell cycles. Semidefined proteose-peptone-based medium were inoculated to a density of 2500 cells/ml with log-growth-phase ciliates in the presence of the test material in DMSO. The test material was evaluated in each of three replicates at 6-8 different concentrations. Controls were inoculated with T. pyriformis in the absence of test material. Following incubation at 27 C, the population density of T. pyriformis was measured at 540 nM. The 50% growth inhibitory concentration was determined from probit analysis of absorbance values and concentrations.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	40-hr IGC50 = 5.76 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	Yes, Probit Anaylsis (Finney, 1971)

Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 2-undecanone required for 50% growth inhibition of Tetrahymena pyriformis is 5.76 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. (1997) TETRATOX: Tetrahymena pyriformis population growth impairment endpoint-asurrogate for fish lethality. Toxicology Methods, 7, 289-309.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, 5-, or 6-undecanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	2000
Species/Strain/Supplier	Green algae
Endpoint basis	
Exposure period (duration)	96 hours
Analytical monitoring	
Remarks for Test Conditions	Based on: log KOW = 4.80, water solubility = 90 mg/L
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	
NOEC, LOEC or NOEL, LOEL	96-hr EC50 = 2.701 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	

Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Calculated data for 2-, 3-, 4-, 5-, or 6-dodecanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	2000
Species/Strain/Supplier	Green algae
Endpoint basis	
Exposure period (duration)	96 hours
Analytical monitoring	
Remarks for Test Conditions	Based on: log KOW = 4.80, water solubility = 90 mg/L
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	
NOEC, LOEC or NOEL, LOEL	96-hr EC50 =1.077 mg/L
Biological observations	
Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	

Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	
Method/guideline	TETRATOX Assay
Test Type	48 hr IGC50 test
GLP	No
Year	1997
Species/Strain/Supplier	Tetrahymena pyriformis/GL-C
Endpoint basis	
Exposure period (duration)	40 hour
Analytical monitoring	GC
Remarks for Test Conditions	A 40 hour static assay was conducted to measure the 50% growth inhibitory concentration of the test substance on Tetrahymena pyriformis. The test was allowed to run through 8-9 cell cycles. Semi-defined proteose-peptone-based medium were inoculated to a density of 2500 cells/ml with log-growth-phase ciliates in the presence of the test material in DMSO. The test material was evaluated in each of three replicates at 6-8 different concentrations. Controls were inoculated with T. pyriformis in the absence of test material. Following incubation at 27 C, the population density of T. pyriformis was measured at 540 nM. The 50% growth inhibitory concentration was determined from probit analysis of absorbance values and concentrations.
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	
Endpoint value	
NOEC, LOEC or NOEL, LOEL	40-hr IGC50 = 4.19 mg/L
Biological observations	
Control response	

satisfactory	
Appropriate statistical evaluations	Yes, Probit Anaylsis (Finney, 1971)
Remarks fields for results	
Conclusion remarks	Under conditions of the experiment the concentration of 2-dodecanone required for 50% growth inhibition of Tetrahymena pyriformis is 4.19 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Schultz, T.W. (1997) TETRATOX: Tetrahymena pyriformis population growth impairment endpoint-asurrogate for fish lethality. Toxicology Methods, 7, 289-309.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Calculated data for 3,3-, 2,3-, 2,4-, or 2,6-dimethylcyclohexanone are equivalent.
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	2000
Species/Strain/Supplier	Green algae
Endpoint basis	
Exposure period (duration)	96 hours
Analytical monitoring	
Remarks for Test Conditions	Based on: log KOW = 4.80, water solubility = 90 mg/L
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	
NOEC, LOEC or NOEL, LOEL	96-hr EC50 =62.67 mg/L
Biological observations	
Control response	

satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for structurally related substance 2-hexanone, 5-methyl-, purity 99.8%.
Method/guideline	OECD: TG-201
Test Type	Growth inhibition of algae
GLP	Yes
Year	2001
Species/Strain/Supplier	Selenastrum capricornutum
Endpoint basis	Cell concentrations and growth rate
Exposure period (duration)	72 hours
Analytical monitoring	Temp., light intensity, rpm, test substance
Remarks for Test Conditions	
Nominal concentrations as mg/L	12.5, 25, 50, 100 and 200
Measured concentrations as mg/L	6.2, 11.9, 22.1, 42.7, 86.3 mg/L
Unit	
Endpoint value	0-72 hr - EbC50 was 75.5 mg/L; ErC50 was 98.2 mg/L
NOEC, LOEC or NOEL, LOEL	72 hour NOEC was estimated to be 42.7 mg/L
Biological observations	No deformed cells were noted
Control response satisfactory	Yes
Appropriate statistical evaluations	

Remarks fields for results	A mean illumination of 741 +/- 1.7 foot-candles was maintained. The mean temperature was 24 deg C and pH ranged from 7.3-7.7. Cultures were oscillated at 100 rpm. The significant loss (up to 82% over the course of the study) in the material was attributed t volatilization. No protocol deviations were noted.
Conclusion remarks	The 72-hour EbC50 and ErC50 values indicate that the test substance would be classified as "harmful to aquatic organisms" according to the European Union's labelling directive and would be classified in a "moderate concern level" according to US EPA's.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Eastman Kodak Co. (2001a) A growth inhibition test with alga, Selenastrum capricornutum. Enviromental Sciences Section, Health and Environment Laboratories, Eastman Kodak Co., Rochester, NY.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	
Method/guideline	ECOSAR
Test Type	Calculated
GLP	
Year	2000
Species/Strain/Supplier	Green algae
Endpoint basis	
Exposure period (duration)	96 hours
Analytical monitoring	
Remarks for Test Conditions	Based on: log KOW = 4.80, water solubility = 90 mg/L
Nominal concentrations as mg/L	
Measured concentrations as mg/L	
Unit	mg/L
Endpoint value	
NOEC, LOEC or NOEL, LOEL	96-hr EC50 =46.902 mg/L
Biological observations	

Control response satisfactory	
Appropriate statistical evaluations	
Remarks fields for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Calculated.
References	ECOSAR EPI Suite (2000) US Environmental Protection Agency.
CAS	123-18-2
Substance Name	2,6,8-Trimethyl-4-nonanone (IBHK)
Remarks for Substance	Assay: 91+%
Method/guideline	OECD Guideline No. 201, Algal Growth Inhibition Test. Directive 92/69/EEC C.3: Algal Inhibition Test. EPA OTS 797.1500, Algal Acute Toxicity Test
Test Type	96-hour acute toxicity test
GLP	Yes
Year	2003
Species/Strain/Supplier	Pseudokirchneriella subcapitata
Endpoint basis	
Exposure period (duration)	96 hours
Analytical monitoring	GC
Remarks for Test Conditions	Nominal concentrations of IHBK were used for all calculations. The EC50 values were not calculated due to less than 50% effect at both 72 and 96 hours. The cell density, growth rate and biomass data was tested for normality and homogeneity of variance using the Shapiro-Wilk's Test and the Bartlett's Test, respectively. As all the data at both time points met the criteria for homogeneity and normality, additional statistical tests, analysis of variance and Dunnett's test, were performed to determine NOEC values. This study evaluated effects of the test substance on growth of the green alga, Pseudokirchnedella subcapitata, over a 96-hour exposure period under static conditions. In the range-finding test of nominal concentrations 0.100, 1.00, 10.0 and 100 mg/L, the percent inhibition was -5, -11, 12, and 28% after 96 hours of exposure. Based on this, the 4-day ECS0 value was > lOOmg IBHK/L. The dose levels selected for the definitive test were 3.13, 6.25, 12.5, 25.0, 50.0, and 100 mg IBHK/L algal assay medium (AAM). IBHK exhibited poor solubility in AAM, so a saturated stock solution at a nominal concentration of 1000 mg IBHK/L AAM was made and the test solutions were dilutions of the stock. Negative control solutions (medium only) were also maintained

concurrently. All test solutions were adjusted for 91.3% purity. Test vessels were 250-mL Erlenmeyer flasks with Shimadzu closure and contained 100 mL of test solution. Each of four replicates per treatment and control were inoculated with 3-7 day old algal culture to achieve 10,000 cells/mE Treatment and control solutions were incubated in a growth chamber at 24 ± 2°C under continuous illumination at 8000 ± 1600 lux. Temperature and pH were recorded at test initiation and termination. Cell numbers were measured daily by electron particle counting. Cell density, biomass (as area under the growth curve) and growth rate were calculated from cell counts.

Nominal concentrations as mg/L 3.13, 6.25, 12.5, 25.0, 50.0, and 100 mg IBHK/L

Measured concentrations as mg/L

Unit

Endpoint value

NOEC, LOEC or NOEL, LOEL 96-hour EC50=1.03 mg/L

Biological observations

Control response satisfactory

Appropriate statistical evaluations Yes

Remarks fields for results

Test Endpoint	Hours	EC50 (mg/L)	NOEC
Cell Density	72	>1.03 mg/L	1.03
Cell Density	96	>1.03 mg/L	1.03
Biomass *	72	>1.03 mg/L	1.03
Biomass *	96	>1.03 mg/L	1.03
Growth Rate	0-72	>1.03 mg/L	1.03
Growth Rate	0-96	>1.03 mg/L	1.03

*Biomass = area under the growth curve

Conclusion remarks No effects were seen at the highest measured test concentration (1.03 mg IBHK/L), which was likely below the water or media solubility of IBHK. This test provides adequate data to assess the risk of IBHK to aquatic algal species

Data Qualities Reliabilities Reliability code 1. Reliable without restriction.

Remarks for Data Reliability Code 1. Guideline study.

References Dow Chemical (2003) Acute toxicity of 2,6,8-trimethyl-4-nonanone in Pseudokirchneriella subcapitata. Unpublished Report.

4 HUMAN HEALTH TOXICITY

4.1 Acute Toxicity

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	
Method/guideline	
Test Type	Acute Oral Toxicity LD 50
GLP	No
Year	1986
Species/Strain	Mice/ddY
Sex	Male
# of animals per sex per dose	4 per dose
Vehicle	Olive Oil
Route of administration	Oral-Gavage
Remarks for test conditions	The acute oral LD 50 was determined using 4 male dd Y mice (24-27 g) per dose. Mice were pre-treated with an intraperitoneal injection of olive oil. Tests were conducted with four concentrations.
Value LD50 or LC50 with confidence limits	7879 gm/kg (95 % CI, 5538-9552 mg/kg) 5465-9535 mg/kg/kg
Number of deaths at each dose level	Not given
Remarks for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Tanii, H., Tsuji, H., Hashimoto, K. (1986) Structure -Toxicity Relationship of Monoketones. Toxicology Letters, 30(1), 13-17.

CAS	821-55-6
Substance Name	2-Nonanone

Remarks for Substance	Assay greater than 95%
Method/guideline	Litchfield and Wilcoxon, 1949
Test Type	Acute Oral Toxicity LD 50
GLP	Yes
Year	1980
Species/Strain	Rat
Sex	Male
# of animals per sex per dose	10
Vehicle	None
Route of administration	Oral-Gavage
Remarks for test conditions	The rats were observed once daily for 14 days. Mortality, toxicity, and pharmacological effects were recorded.
Value LD50 or LC50 with confidence limits	Greater than 5000 mg/kg
Number of deaths at each dose level	1/10
Remarks for results	9/10 rats survived and oral dose of 5.0 g/kg. Toxic signs included lethargy, ataxia prostration, flaccid muscle tone, ptosis and tachypnea. Internal Organs appeared normal on superficial examination, except for lung, heart, and gastrointestinal abnormalities noted in one animal death.
Conclusion remarks	Study conducted in Accordance with FDA's Good Laboratory Practices, 1979
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Moreno O. (1980) Acute Toxicity Studies. Project No. MB80-4817A. Unpublished report to RIFM.

CAS	925-78-0
Substance Name	3-Nonanone
Remarks for Substance	
Method/guideline	
Test Type	Acute Oral Toxicity
GLP	No
Year	1967

Species/Strain	Mouse/CF-1
Sex	Male and Female
# of animals per sex per dose	10/group
Vehicle	None
Route of administration	Oral-Gavage
Remarks for test conditions	Male and female CF-1 mice weighing 17-25 grams were given a single oral dose of the test substance and observed for 72 hours.
Value LD50 or LC50 with confidence limits	5270 mg/kg (CI, =/- 542.5 mg/L kg
Number of deaths at each dose level	Not given
Remarks for results	
Conclusion remarks	The acute oral LD50 of 3-nonanone in CF-1 mice is 5270 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Hoffman-LaRoche (1967) Acute toxicity, eye, and skin irritation tests of fragrance materials. Unpublished Report to the Research Institute for Fragrance Materials.
CAS	693-54-9
Substance Name	2-Decanone
Remarks for Substance	
Method/guideline	
Test Type	Acute Oral Toxicity LD 50
GLP	No
Year	1986
Species/Strain	Mice/ddY
Sex	Male
# of animals per sex per dose	4 per dose
Vehicle	Olive Oil
Route of administration	Oral-Gavage
Remarks for test conditions	The acute oral LD 50 was determined using 4 male dd Y mice (24-27 g) per dose. Mice were pre-treated with an

	intraperitoneal injection of olive oil. Tests were conducted with four concentrations.
Value LD50 or LC50 with confidence limits	7940 gm/kg (95 % CI, 3847- 16317 mg/kg) 5465-9535 mg/kg/kg 5465-9535 mg/kg/kg
Number of deaths at each dose level	Not given
Remarks for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Tanii, H., Tsuji, H., Hashimoto, K. (1986) Structure -Toxicity Relationship of Monoketones. Toxicology Letters, 30(1), 13-17.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	
Method/guideline	Litchfield and Wilcoxon, 1949
Test Type	Acute Dermal LD50
GLP	No
Year	1974
Species/Strain	Rabbit
Sex	Not reported
# of animals per sex per dose	4
Vehicle	None
Route of administration	Dermal
Remarks for test conditions	4 Rabbits were used. Animals were observed for mortality and systemic effects over a 14 day period.
Value LD50 or LC50 with confidence limits	Greater than 5000 mg/kg
Number of deaths at each dose level	No deaths
Remarks for results	
Conclusion remarks	The oral LD50 of 2-undecanone in rats exceeds 5000 mg/kg.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.

Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Levenstein I. (1974) Acute toxicity study in rats and rabbits. Unpublished report to RIFM.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	
Method/guideline	Litchfield and Wilcoxon, 1949
Test Type	Acute Oral LD 50
GLP	No
Year	1974
Species/Strain	Rat
Sex	Not reported
# of animals per sex per dose	10
Vehicle	None
Route of administration	Oral-Gavage
Remarks for test conditions	10 Rats were used. Animals were observed for mortality and systemic effects over a 14 day period.
Value LD50 or LC50 with confidence limits	Greater than 5000 mg/kg
Number of deaths at each dose level	No Deaths. Gross pathology performed on animals surviving to 14 days revealed no changes that could be associated with administration of the test substance.
Remarks for results	
Conclusion remarks	The oral LD50 of 2-nonanone in rats exceeds 5000 mg/kg.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Levenstein, I. (1974) Acute toxicity study in rats and rabbits. Unpublished report to RIFM.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	

Method/guideline	
Test Type	Acute Oral Toxicity LD 50
GLP	No
Year	1986
Species/Strain	Mice/ddY
Sex	Male
# of animals per sex per dose	4 per dose
Vehicle	Olive Oil
Route of administration	Oral-Gavage
Remarks for test conditions	The acute oral LD 50 was determined using 4 male dd Y mice (24-27 g) per dose. Mice were pre-treated with an intraperitoneal injection of olive oil. Tests were conducted with four concentrations.
Value LD50 or LC50 with confidence limits	19448 gm/kg (95 % CI, 11900-31790 mg/kg) 5465-9535 mg/kg/kg 5465-9535 mg/kg/kg
Number of deaths at each dose level	Not given
Remarks for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Tanii, H., Tsuji, H., Hashimoto, K. (1986) Structure -Toxicity Relationship of Monoketones. Toxicology Letters, 30(1), 13-17.
CAS	6175-49-1
Substance Name	2-Dodecanone
Remarks for Substance	Data are for homologue, 2-tridecanone.
Method/guideline	
Test Type	Acute Toxicity
GLP	Yes
Year	2000
Species/Strain	Rat/Sprague-Dawley
Sex	Male and Female

# of animals per sex per dose	5
Vehicle	Olive oil
Route of administration	Oral-Gavage
Remarks for test conditions	Male and female rats, 161-191 gm body weight, were administered the test compound neat and observed regularly for 24 hours and then daily for the next 14 days. At the conclusion of the study all animals were sacrificed and subjected to gross pathological
Value LD50 or LC50 with confidence limits	Greater than 2000 mg/kg
Number of deaths at each dose level	
Remarks for results	No deaths or effects in either sex
Conclusion remarks	The oral LD50 of 2-tridecanone in rats exceeds 2000 mg/kg.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Dragoco Gerberding and Co. GmbH (2000) Acute toxicity study of 2-tridecanone by oral administration to Sprague-Dawley rats. Unpublished report.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related substance, 3,5,5-trimethylcyclohexenone.
Method/guideline	Wilcoxon & Litchfield method
Test Type	Acute Oral LD50
GLP	No
Year	1982
Species/Strain	Rat/Sprague-Dawley albino
Sex	Male
# of animals per sex per dose	5
Vehicle	None
Route of administration	Oral
Remarks for test conditions	Test substance(s) were administered to 6 groups of five male albino Sprague-Dawley animals. Animals were fasted 3 to 4 hours prior to dosing. Animals were observed at 1, 4, 24 hours

	immediately after compound administration and once daily thereafter for a total of 14 days. Necropsy was conducted.
Value LD50 or LC50 with confidence limits	3450 mg/kg
Number of deaths at each dose level	
Remarks for results	Animals exhibited depression, ptosis, lacrimation, labored respiration & evidence of excessive urination. Congestion of lungs, kidneys, adrenals, & pancreas and gastrointestinal inflammation were observed.
Conclusion remarks	The acute oral LD50 of 3,5,5-trimethylcyclohexenone in rats is 3450 mg/kg.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Exxon Chemical Americas (1982) Unpublished report to Environmental Protection Agency.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related substance, 3,5,5-trimethylcyclohexenone
Method/guideline	Wilcoxon & Litchfield method
Test Type	Acute Inhalation toxicity
GLP	No
Year	1982
Species/Strain	Rat/Wistar
Sex	Male
# of animals per sex per dose	10
Vehicle	None
Route of administration	Inhalation
Remarks for test conditions	Groups of 10 male Wistar animals were exposed to various doses of test material. Each exposure was for 4 hours. Animals were observed approximately every 30 minutes for toxic signs and death. Following exposure animals were observed daily for 14 days for toxic signs and death. Gross necropsies were performed.
Value LD50 or LC50 with confidence limits	7 mg/L (1281 ppm)

Number of deaths at each dose level	
Remarks for results	Animals exhibited dyspnea, piloerection, depression, & decreased activity.
Conclusion remarks	The acute inhalation LD50 of 3,5,5-trimethylcyclohexenone in Wistar rats is 7 mg/L.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Exxon Chemical Americas (1982) Unpublished report to Environmental Protection Agency.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for dehydro derivative, 6-methyl-5-hepten-2-one.
Method/guideline	
Test Type	Acute Oral Toxicity LD 50
GLP	No
Year	1972
Species/Strain	Rat
Sex	Not reported
# of animals per sex per dose	10
Vehicle	None
Route of administration	Oral-Gavage
Remarks for test conditions	
Value LD50 or LC50 with confidence limits	4100 mg/kg (95% CI, 3330-5040 mg/kg)
Number of deaths at each dose level	
Remarks for results	Symptomatology: Immediate stimulation followed by ataxia
Conclusion remarks	The acute oral LD50 of 6-methyl-5-hepten-2-one in rats is 4100 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Keating J. (1972) Acute oral toxicity in rats, dermal toxicity in rabbits. Unpublished report to RIFM dated June 7, 1972.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for dehydro derivative, 6-methyl-5-hepten-2-one.
Method/guideline	
Test Type	Acute Dermal Toxicity LD 50
GLP	No
Year	1972
Species/Strain	Rabbit
Sex	Not reported
# of animals per sex per dose	6
Vehicle	None
Route of administration	Dermal
Remarks for test conditions	6 Rabbits per dose were used. Animals were observed for mortality and clinical signs over a period of 14 days.
Value LD50 or LC50 with confidence limits	Greater than 5000 mg/kg
Number of deaths at each dose level	
Remarks for results	1/6 Deaths. Death occurred on day 9. Acute dermal LD 50 greater than 5000 mg/kg.
Conclusion remarks	The dermal LD50 of 6-methyl-5-hepten-2-ne in rabbis is greater than 5000 mg/kg.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Keating J. (1972) Acute oral toxicity in rats, dermal toxicity in rabbits. Unpublished report to RIFM dated June 7, 1972.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data for dehydro derivative, 6-methyl-5-hepten-2-one
Method/guideline	
Test Type	Acute Inhalation toxicity
GLP	No

Year	1974
Species/Strain	Rat
Sex	Not reported
# of animals per sex per dose	12
Vehicle	None
Route of administration	Inhalation
Remarks for test conditions	Air was passed through a 5-cm thick layer of the chemical. Atmosphere was saturated with steam at 20 C. 12 animals were exposed for 8 hours and observed.
Value LD50 or LC50 with confidence limits	No effects to an atmosphere saturated with the test material at 20 C.
Number of deaths at each dose level	0/12 deaths were observed
Remarks for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 4. Not assignable.
Remarks for Data Reliability	Code 4. Only short abstract available.
References	BASF (1974) Acute toxicity studies on 6-methyl-5-hepten-2-one. Unpublished report.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for dehydro derivative, 6-methyl-5-hepten-2-one.
Method/guideline	
Test Type	Acute Oral LD50
GLP	No
Year	1974
Species/Strain	Rat
Sex	Not reported
# of animals per sex per dose	10
Vehicle	None
Route of administration	Oral-Gavage

Remarks for test conditions	The approximate peroral LD 50 in rats was determined
Value LD50 or LC50 with confidence limits	Greater than 4200 ul/kg
Number of deaths at each dose level	0/12
Remarks for results	
Conclusion remarks	The oral LD50 of 6-methyl-5-hepten-2-one in rats is greater than 4200 ul/kg.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	BASF (1974) Acute toxicity studies on 6-methyl-5-hepten-2-one. Unpublished report.

4.2 Genetic Toxicity

4.2.1 *In vitro* Genotoxicity

CAS	4485-09-0
Substance Name	4-Nonanone
Remarks for Substance	Data are for isomer, 2,6-dimethyl-4-heptanone.
Method/guideline	Ames Test
Test Type	Reverse mutation
System of Testing	Bacterial
GLP	No
Year	1986
Species/Strain	Salmonella typhimurium TA 100, TA98, TA97, TA1535, and TA1537
Metabolic Activation	Male Sprague Dawley rat liver microsome fraction S9 from Aroclor induced rats.
Doses/concentration levels	1-333 ug per plate
Statistical Methods	Not given
Remarks for test conditions	After 48-hour incubation at 37 C, each assay plate was counted. Routine positive control plates were prepared: sodium azide for TA1535 and TA100, 4-nitro-o-phenylenediamine for

	TA98, and 9-aminoacridine for TA97 and TA1537, 2-aminoanthracen.
Result	No mutagenic effects
Cytotoxic concentration	
Genotoxic effects	None
Appropriate statistical evaluations	None given
Remarks for results	
Conclusion remarks	No mutagenic activity of 2,6-dimethyl-4-heptanone was observed using Salmonella typhimurium strains TA98, TA100, TA1535 & TA1538 in the presence or absence of S9 fraction.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Mortelmans, K., Haworth, S., Lawlor, T., Speck, W., Tainer, B and Zeiger, E. (1986) Salmonella Mutagenicity Tests: II. Results from the Testing of 270 Chemicals. Environmental Mutagenesis 8(Supplement 7): 1-119.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Data are for homologous ketone, 6,10-dimethyl-2-undecatrienone.
Method/guideline	Ames Test
Test Type	Reverse mutation
System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535 & TA1537
Metabolic Activation	With and without S9 fraction rat liver treated with Aroclor 1254
Doses/concentration levels	3 micromol/plate , then at 0.03, 0.3, 3, and 30 umole/plate
Statistical Methods	Not given
Remarks for test conditions	The solvent used was ethanol. Only one replicate was performed for the substances which tested negative. Similar to OECD 471. No E. coli strain was included.
Result	No mutagenic effects at any concentration.

Cytotoxic concentration	Not given
Genotoxic effects	None
Appropriate statistical evaluations	None given
Remarks for results	
Conclusion remarks	No mutagenic activity of 6,10-dimethyl-2-undecatrienone was observed using Salmonella typhimurium strains TA98, TA100, TA1535 & TA1538 in the presence or absence of S9 fraction.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Florin, I., Rutberg, L., Curvall, M. and Enzell, C. R. (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames' test. Toxicology 18: 219-232.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data are for homologous ketone, tetramethylethylcyclohexanone.
Method/guideline	Ames Test
Test Type	Reverse mutation
System of Testing	Bacterial
GLP	No
Year	1983
Species/Strain	Salmonella typhimurium TA100, TA98, TA1535, and TA1537
Metabolic Activation	With and without rat liver microsome fraction S9 from Aroclor induced rats.
Doses/concentration levels	up to 3.6 mg/plate
Statistical Methods	Method of Kastenbaum and Bowman (1970)
Remarks for test conditions	Positive controls were run in each experiment with the reference mutagens sodium azide and benzo(a)pyrene
Result	No mutagenic effects
Cytotoxic concentration	Not given
Genotoxic effects	None
Appropriate statistical evaluations	None given
Remarks for results	

Conclusion remarks	No mutagenic effects
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Wild, D., King, M.-T., Gocke, E. and Eckhardt, K. (1983) Study of Artifical Flavouring Susbtances for Mutagenicity in the Salmonella/Microsome, BASC and Micronucleus Tests. Fd. Chem. Toxic. 21(6): 707-719.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for homologous ketone, 2,2,6-trimethylcyclohexanone
Method/guideline	Ames Test
Test Type	Reverse mutation
System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98 and TA100
Metabolic Activation	With and without S9 fraction rat liver treated with Aroclor 1254
Doses/concentration levels	3 micromol/plate , then at 0.03, 0.3, 3, and 30 umole/plate
Statistical Methods	Not given
Remarks for test conditions	The solvent used was ethanol. Only one replicate was performed for the substances which tested negative. Similar to OECD 471. No E. coli strain was included.
Result	No mutagenic effects at any concentration.
Cytotoxic concentration	
Genotoxic effects	None
Appropriate statistical evaluations	None given
Remarks for results	
Conclusion remarks	No mutagenic activity of 2,2,6-trimethylcyclohexanone was observed using Salmonella typhimurium strains TA98and TA100.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.

References	Florin, I., Rutberg, L., Curvall, M. and Enzell, C. R. (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames' test. Toxicology 18: 219-232.
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for isomer structurally related ketone, 3,5,5-dimethylcyclohexenone.
Method/guideline	Ames Test
Test Type	Reverse mutation
System of Testing	Bacterial
GLP	No
Year	1986
Species/Strain	Salmonella typhimurium TA 100, TA98, TA1535, and TA1537
Metabolic Activation	Male Sprague Dawley rat liver microsome fraction S9 from Aroclor induced rats.
Doses/concentration levels	1-10,000 ug per plate
Statistical Methods	Not given
Remarks for test conditions	After 48-hour incubation at 37 C, each assay plate was counted. Routine positive control plates were prepared: sodium azide for TA1535 and TA100, 4-nitro-o-phenylenediamine for TA98, and 9-aminoacridine for TA97 and TA1537, 2-aminoanthracen
Result	No mutagenic effects
Cytotoxic concentration	
Genotoxic effects	None
Appropriate statistical evaluations	None given
Remarks for results	
Conclusion remarks	No mutagenic activity was observed upon incubation of 3,5,5-trimethylcyclohexenone with Salmonella typhimurium strains TA98, TA100, TA1535 & TA1538 in the presence or absence of S9 fraction.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Mortelmans, K., Haworth, S., Lawlor, T., Speck, W., Tainer, B and Zeiger, E. (1986) Salmonella Mutagenicity Tests: II. Results from the Testing of 270 Chemicals. Environmental

Mutagenesis 8(Supplement 7): 1-119.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for homologous ketone, 6-methyl-5-hepten-2-one.
Method/guideline	Ames Test
Test Type	Reverse mutation
System of Testing	Bacterial
GLP	No
Year	1980
Species/Strain	Salmonella typhimurium strains TA98, TA100, TA1535 & TA1537
Metabolic Activation	With and without S9 fraction rat liver treated with Aroclor 1254
Doses/concentration levels	3 micromol/plate , then at 0.03, 0.3, 3, and 30 umole/plate
Statistical Methods	Not given
Remarks for test conditions	The solvent used was ethanol. Only one replicate was performed for the substances which tested negative. Similar to OECD 471. No E. coli strain was included.
Result	No mutagenic effects at any concentration.
Cytotoxic concentration	
Genotoxic effects	None
Appropriate statistical evaluations	None given
Remarks for results	
Conclusion remarks	No mutagenic activity of 6-methyl-5-hepten-2-one was observed using Salmonella typhimurium strains TA98, TA100, TA1535 & TA1538 in the presence or absence of S9 fraction.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Florin, I., Rutberg, L., Curvall, M. and Enzell, C. R. (1980) Screening of tobacco smoke constituents for mutagenicity using the Ames' test. Toxicology 18: 219-232.

4.2.2 *In vivo* Genotoxicity

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data for structurally related ketone, 3,5,5-trimethylcyclohexenone
Method/guideline	
Test Type	Clastogenicity assay
GLP	Ambiguous
Year	1988
Species/Strain	Mouse/CD-1
Sex	Male and Female
Route of administration	Intraperitoneal
Doses/concentration levels	0.54 ml/kg
Exposure period	48 hours
Remarks for test conditions	Groups of male and female CD-1 mice were given a single oral dose of the test material in corn oil and sacrificed at 12, 24 and 48 hours. A positive control group was given 0.25 ml/kg of triethylene melamine. Bone marrow from the femur was aspirated into a syringe containing fetal calf serum Bone marrow preparations were stained and 1000 polychromatic erythrocytes were scored for the presence of micronuclei. Micronucleased normocytes were also scored.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	The mean number of micronucleated PE/1000 PE at 0 and 48 hours. At 540 mg/kg, males, 7/5000 and females, 6/5000. Controls; males, 4/5000 and females, 6/5000
Genotoxic effects	No clastogenic effects
NOEL (C)/ LOEL (C)	540 uL/kg (498 mg/kg)
Appropriate statistical evaluations	One-way analysis of variance and Duncan's multiple range test
Remarks for results	
Conclusion remarks	Under conditions of the study, 3,5,5-trimethylcyclohexenone is not clastogenic.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	O'Donoghue J.L., Haworth S.R., Curren R.D., Kirby P.E., Lawlor T., Moran E.J., Phillips R.D., Putnam D.L., Rogers-Back A.M., Slesinski R.S., and Thilagar A. (1988) Mutagenicity

	studies on ketone solvents: Methyl ethyl ketone, methyl isobutyl ketone, and i
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data for structurally related ketone, 3,5,5-trimethylcyclohexenone, 97.2%, chemical assay.
Method/guideline	Drosophila mutagenicity assay
Test Type	Drosophila mutagenicity assay
GLP	Yes
Year	1994
Species/Strain	Drosophila melanogaster/Basc females
Sex	Male and Female
Route of administration	Injection
Doses/concentration levels	0 or 12,500 mg/kg
Exposure period	72 hours
Remarks for test conditions	Two to three discs were saturated with the test substance in 5% sucrose solution. Solutions were renewed at 24 and 48 hr. After 72 hrs surviving males were mated. Each male was mated with three Basc virgin females every two to three days to three broods. No more than 100 F1 females were mater over the three broods with P1 males. F2 cultures were scored as presumptive lethals if the number of wild-type males was 0, 1, or less than 5% of the number of Basc males. All putative lethals were confirmed through an additional generation. If the feeding test was nonmutagenic, 2-3 day old CantorS males were injected with 0.7% saline solution containing the test substance.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	Lethals for Broods 1,2, and 3: At 12500 mg/kg; 0/2282, 10/1837, and 2/1445. At 0 mg/kg, 0/1855, 8/2013, and 2/1887. % Lethals at 2000 and mg/kg: 0.22% and 0.17%
Genotoxic effects	No mutagenic effects
NOEL (C)/ LOEL (C)	12,500 mg/kg
Appropriate statistical evaluations	Yes (Kasenbaum and Bowen, 1970)
Remarks for results	Under conditions of the test, 3,5,5-trimethylcyclohexenone is not mutageni.c
Conclusion remarks	Under conditions of the test, 3,5,5-trimethylcyclohexenone is not mutageni.c
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.

Remarks for Data Reliability	Code 1. Guideline study.
References	Foureman P., Mason J.M., Valencia R. and Zimmering S. (1994) Chemical Mutagenesis testing in Drosophila. X. Results of 70 coded chemicals tested for the National Toxicology Program. Environmental and Molecular Mutagenesis 23, 208-227.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data for structurally related ketone, 3,5,5-trimethylcyclohexenone, 97.2%, chemical assay.
Method/guideline	Drosophila mutagenicity assay
Test Type	Drosophila mutagenicity assay
GLP	Yes
Year	1994
Species/Strain	Drosophila melanogaster/Basc females
Sex	Male and Female
Route of administration	Oral-Diet
Doses/concentration levels	0 or 2000 mg/kg
Exposure period	72 hours
Remarks for test conditions	Two to three discs were saturated with the test substance in 5% sucrose solution. Solutions were renewed at 24 and 48 hr. After 72 hrs surviving males were mated. Each male was mated with three Basc virgin females every two to three days to three broods. No more than 100 F1 females were mater over the three broods with P1 males. F2 cultures were scored as presumptive lethals if the number of wild-type males was 0, 1, or less than 5% of the number of Basc males. All putative lethals were confirmed through an additional generation. If the feeding test was nonmutagenic, 2-3 day old CantorS males were injected with 0.7% saline solution containing the test substance.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	Lethals for Broods 1,2, and 3: At 2000 mg/kg; 1/2281, 4/2077, and 2/2185. At 0 mg/kg, 4/2184, 4/1852, and 3/2087. % Lethals at 2000 and) mg/kg: 0.11% and 0.18%
Genotoxic effects	No mutagenic effects
NOEL (C)/ LOEL (C)	2000 mg/kg
Appropriate statistical evaluations	Yes (Kasenbaum and Bowen, 1970)
Remarks for results	Under conditions of the test, 3,5,5-trimethylcyclohexenone is not mutagenic

Conclusion remarks	Under conditions of the test, 3,5,5-trimethylcyclohexenone is not mutagenic
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Foureman P., Mason J.M., Valencia R. and Zimmering S. (1994) Chemical Mutagenesis testing in Drosophila. X. Results of 70 coded chemicals tested for the National Toxicology Program. Environmental and Molecular Mutagenesis 23, 208-227.
CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related alkyl-substituted cycloalkanone, 2-hexylidenecyclopentanone.
Method/guideline	Micronucleus test (Schmid, 1976)
Test Type	Clastogenicity assay
GLP	Ambiguous
Year	1983
Species/Strain	Mouse/NMRI
Sex	Male and Female
Route of administration	Intraperitoneal
Doses/concentration levels	
Exposure period	
Remarks for test conditions	Groups of 10- to 14-week-old NMRI mice were intraperitoneally injected at 0 and 24 hours with 333, 666, or 1,000 mg/kg bw. At 30 hours, the mice were killed and bone marrow smears were prepared using the staining method of Schmid (1976).
Effect on mitotic index or PCE/NCE ratio by dose level and sex	The mean number of micronucleated PE/1000 PE at 0, 500, 333, and 180 mg/kg bw was 2.0, 2.0, 1.9, and 1.2, respectively.
Genotoxic effects	None
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	Yes. Statistical significance determined by methods of Kastenbaum and Bowman (1970).
Remarks for results	The test substance did not induce micronuclei in this assay.
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.

Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Wild D., King, M.T., Gocke, E. and Eckhardt, K. (1983) Study of artificial flavouring substances for mutagenicity in the salmonella/microsome, basc and micronucleus tests. Fd Chem Toxicol., 21(6), 707-719.
CAS	13395-76-1
Substance Name	2,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related alkyl-substituted cycloalkanone, 2-hexylidenecyclopentanone.
Method/guideline	Sex linked recessive lethal mutation assay (Wuergler et al., 1977)
Test Type	Sex-linked lethal assay
GLP	Ambiguous
Year	1983
Species/Strain	Drosophila melanogaster
Sex	Not reported
Route of administration	Oral-Diet
Doses/concentration levels	5mM
Exposure period	
Remarks for test conditions	Flies were exposed to the test compound prepared in a 5% saccharose solution and 2% ethanol and 2% Tween 80 for compounds with poor water solubility. Further details of the methodology were not reported.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	No (%) of sex-linked lethals/chromosomes tested: Brood 1, 4/1191 (0.34%); Brood 2 , 3/1112 (0.27%);Brood 3, 3/1201 (0.25%); Controls: Brood 1, 0.23%; Brood 2, 0.19%; Brood 3, 0.29%
Genotoxic effects	
NOEL (C)/ LOEL (C)	5 mM
Appropriate statistical evaluations	Yes. Statistical significance determined by methods of Kastenbaum and Bowman (1970).
Remarks for results	The test substance did not increase the number of sex-linked recessive lethal mutations as compared to controls.
Conclusion remarks	The test substance did not induce sex linked recessive lethals in Drosophila melanogaster.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report

	which meets basic scientific principles.
References	Wild D., King, M.T., Gocke, E. and Eckhardt, K. (1983) Study of artificial flavouring substances for mutagenicity in the salmonella/microsome, basc and micronucleus tests. Fd Chem Toxicol., 21(6), 707-719.
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related alkyl-substituted cyclohexanone, tetramethylethylcyclohexanone.
Method/guideline	Micronucleus test (Schmid, 1976)
Test Type	Clastogenicity assay
GLP	Ambiguous
Year	1983
Species/Strain	Mouse/NMRI
Sex	Male and Female
Route of administration	Intraperitoneal
Doses/concentration levels	
Exposure period	
Remarks for test conditions	Groups of 10- to 14-week-old NMRI mice were intraperitoneally injected at 0 and 24 hours with 333, 666, or 1,000 mg/kg bw. At 30 hours, the mice were killed and bone marrow smears were prepared using the staining method of Schmid (1976).
Effect on mitotic index or PCE/NCE ratio by dose level and sex	The mean number of micronucleated PE/1000 PE at 0, 450, 307, and 180 mg/kg bw was 1.3, 1.3, 1.5, and 1.3, respectively.
Genotoxic effects	None
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	Yes. Statistical significance determined by methods of Kastenbaum and Bowman (1970).
Remarks for results	The test substance did not induce micronuclei in this assay.
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Wild D., King, M.T., Gocke, E. and Eckhardt, K. (1983) Study of artificial flavouring substances for mutagenicity in the salmonella/microsome, basc and micronucleus tests. Fd Chem

Toxicol., 21(6), 707-719.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related alkyl-substituted cyclohexanone, tetramethylethylcyclohexanone.
Method/guideline	Sex linked recessive lethal mutation assay (Wuergler et al., 1977)
Test Type	Sex-linked lethal assay
GLP	Ambiguous
Year	1983
Species/Strain	Drosophila melanogaster
Sex	Not reported
Route of administration	Oral-Diet
Doses/concentration levels	10mM
Exposure period	
Remarks for test conditions	Flies were exposed to the test compound prepared in a 5% saccharose solution and 2% ethanol and 2% Tween 80 for compounds with poor water solubility. Further details of the methodology were not reported.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	No (%) of sex-linked lethals/chromosomes tested: Brood 1, 3/1218 (0.25%); Brood 2 , 1/1220 (0.08%);Brood 3, 3/1221 (0.25%); Controls: Brood 1, 0.23%; Brood 2, 0.19%; Brood 3, 0.29%
Genotoxic effects	
NOEL (C)/ LOEL (C)	10 mM
Appropriate statistical evaluations	Yes. Statistical significance determined by methods of Kastenbaum and Bowman (1970).
Remarks for results	The test substance did not increase the number of sex-linked recessive lethal mutations as compared to controls.
Conclusion remarks	The test substance did not induce sex linked recessive lethals in Drosophila melanogaster.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Wild D., King, M.T., Gocke, E. and Eckhardt, K. (1983) Study of artificial flavouring substances for mutagenicity in the salmonella/microsome, basc and micronucleus tests. Fd Chem Toxicol., 21(6), 707-719.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexyl alcohol, 2-isopropyl-5-methylcyclohexanol (dl-menthol).
Method/guideline	
Test Type	Dominant lethal assay-Acute study
GLP	No
Year	1975
Species/Strain	Rat/Random bred
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	Test 1: 1.45, 14.5, or 145 mg/kg bw; test 2: 500 or 3000 mg/kg bw
Exposure period	Single dose
Remarks for test conditions	Groups of male rats were gavaged with 1.45, 14.5 or 145 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 1) or 500 or 3000 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 2). Male rats were mated with 2 female rats per week for 8 weeks. 14 days after ma
Effect on mitotic index or PCE/NCE ratio by dose level and sex	
Genotoxic effects	
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	Under conditions of the study, cyclohexyl alcohol, 2-isopropyl-5-methylcyclohexanol (dl-menthol), produced no evidence of genotoxic effects.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Food and Drug Administration (FDA) (1975) Mutagenic evaluation of compound FDA 71-57, menthol. NTIS PB-245-444 (FDA 71-268).

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexyl alcohol, 2-isopropyl-5-methylcyclohexanol (dl-menthol).
Method/guideline	Chromosomal aberration
Test Type	Cytogenetic assay-Subacute study
GLP	No
Year	1975
Species/Strain	Rat/Albino
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	Test 1: 1.45, 14.5, or 145 mg/kg bw; test 2: 1150 mg/kg bw
Exposure period	Five doses 24 hours apart
Remarks for test conditions	Groups of rats were gavaged with 1.45, 14.5 or 145 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 1) or 500 or 3000 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 2) and groups of rats were killed at 6, 24 and 48 hours. 4 hours after administration and 2 hours prior to termination, rats were intraperitoneally injected with 4 mg colcemid/kg bw. Bone marrow was removed and slides were prepared and analyzed.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	
Genotoxic effects	None
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	2-Isopropyl-5-methylcyclohexanol did not induce chromosomal aberrations.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Food and Drug Administration (FDA) (1975) Mutagenic evaluation of compound FDA 71-57, menthol. NTIS PB-245-444 (FDA 71-268).

CAS	2816-57-1

Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexyl alcohol, 2-isopropyl-5-methylcyclohexanol (dl-menthol).
Method/guideline	Chromosomal aberration
Test Type	Cytogenetic assay-Acute study
GLP	No
Year	1975
Species/Strain	Rat/Albino
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	Test 1: 1.45, 14.5, or 145 mg/kg bw; test 2: 500 or 3000 mg/kg bw
Exposure period	6, 24 or 48 hours
Remarks for test conditions	Groups of rats were gavaged with 1.45, 14.5 or 145 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 1) or 500 or 3000 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 2) and groups of rats were killed at 6, 24 and 48 hours. 4 hours after administration and 2 hours prior to termination, rats were intraperitoneally injected with 4 mg colcemid/kg bw. Bone marrow was removed and slides were prepared and analyzed.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	
Genotoxic effects	None.
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	2-Isopropyl-5-methylcyclohexanol did not induce chromosomal aberrations.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Food and Drug Administration (FDA) (1975) Mutagenic evaluation of compound FDA 71-57, menthol. NTIS PB-245-444 (FDA 71-268).
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone

Remarks for Substance	Data are for structurally related cyclohexyl alcohol, 2-isopropyl-5-methylcyclohexanol (dl-menthol).
Method/guideline	
Test Type	Host-mediated-Subcute study
GLP	No
Year	1975
Species/Strain	Mouse/ICR
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	Test 1: 1.45, 14.5 and 145 mg/kg bw; Test 2:1150 mg/kg bw
Exposure period	Five doses 24 hours apart
Remarks for test conditions	Indicator organisms were Salmonella typhimurium strains G46 and TA1530, and Saccharomyces cervisiae D3. Groups of mice were given 1.45, 14.5 and 145 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 1) or 500 or 5000 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 2) by gavage followed by intraperitoneal injection of 2 ml indicator organism. Three hours later, mice were killed and intraperitoneally injected with 2 ml of sterile saline. As much fluid as possible was removed from the peritoneal cavity and dilutions were made from each exudate. Dilutions were plated and incubated for 18-40 hours. Further dilutions were made, plated and incubated at 30deg C for 40 hours after which bacterial scoring was conducted for calculation of mutation frequency and recombinant frequency.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	
Genotoxic effects	Elevated recombinant frequency in Saccharomyces D3
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	No significant increase in mutant and recombinant frequency at any dose in Salmonella G46 and TA1530, but in Saccharomyces D3 an elevation of recombinant frequency was reported. In vitro tests using same organisms were all negative.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Food and Drug Administration (FDA) (1975) Mutagenic evaluation of compound FDA 71-57, menthol. NTIS PB-245-

444 (FDA 71-268).

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexyl alcohol, 2-isopropyl-5-methylcyclohexanol (dl-menthol).
Method/guideline	
Test Type	Host-mediated-Acute study
GLP	No
Year	1975
Species/Strain	Mouse/ICR
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	Test 1: 1.45, 14.5 and 145 mg/kg bw; Test 2: 500 and 5000 mg/kg bw
Exposure period	Single exposure
Remarks for test conditions	Indicator organisms were Salmonella typhimurium strains G46 and TA1530, and Saccharomyces cervisiae D3. Groups of mice were given 1.45, 14.5 and 145 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 1) or 500 or 5000 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 2) by gavage followed by intraperitoneal injection of 2 ml indicator organism. Three hours later, mice were killed and intraperitoneally injected with 2 ml of sterile saline. As much fluid as possible was removed from the peritoneal cavity and dilutions were made from each exudate. Dilutions were plated and incubated for 18-40 hours. Further dilutions were made, plated and incubated at 30deg C for 40 hours after which bacterial scoring was conducted for calculation of mutation frequency and recombinant frequency.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	
Genotoxic effects	Only at 5000 mg/kg bw in Salmonella TA1530.
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	
Remarks for results	In vitro tests using same organisms were all negative.
Conclusion remarks	No significant increase in mutant and recombinant frequency at any dose in Salmonella G46 and Saccharomyces D3. At the highest dose tested in Salmonella TA1530 a significant

	increase in mutant frequency was reported.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Food and Drug Administration (FDA) (1975) Mutagenic evaluation of compound FDA 71-57, menthol. NTIS PB-245-444 (FDA 71-268).
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexyl alcohol, 2-isopropyl-5-methylcyclohexanol (dl-menthol).
Method/guideline	
Test Type	Micronucleus test
GLP	Ambiguous
Year	1993
Species/Strain	Mouse/B6C3F1
Sex	Male
Route of administration	Intraperitoneal
Doses/concentration levels	0, 250, 500, and 1,000 mg/kg bw
Exposure period	3 daily exposures
Remarks for test conditions	Groups of 5-6 mice were intraperitoneally injected on 3 consecutive days with 1X, 0.5X and 0.25X of the test chemical. A positive control and solvent control were also used. 24 hours after the last treatment, mice were killed, bone marrow removed and slides were prepared. For each mouse, the number of MN-PCE in 2,000 PCE and the percent PCE in 200 erythrocytes were determined.
Effect on mitotic index or PCE/NCE ratio by dose level and sex	0 mg/kg bw: survival=5/5 mice; MN-PCE/1000=2.90; %PCE=54.4 250 mg/kg bw: survival=5/5 mice; MN-PCE/1000=3.60; %PCE=64.2 500 mg/kg bw: survival=5/5 mice; MN-PCE/1000=2.20; %PCE=56.7 1000 mg/kg bw: survival=3/6 mice; MN-PCE/1000=3.67; %PCE=51.8
Genotoxic effects	None
NOEL (C)/ LOEL (C)	
Appropriate statistical evaluations	Yes.

Remarks for results	
Conclusion remarks	2-Isopropyl-5-methylcyclohexanol was negative in the micronucleus test.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions. Part of NTP study program.
References	Shelby, M.D., Erexson, G.L., Hook, G.J., and Tice, R.R. (1993) Evaluation of a three-exposure mouse bone marrow micronucleus protocol: Results with 49 chemicals. Environ Mol Mutagen 21:160-179.

4.3 Repeated Dose Toxicity

CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	
Method/guideline	3-week gavage study
GLP	No
Year	1979
Species/Strain	Rat/Charles River CD
Sex	Male and Female
Route of administration	Oral-Gavage
Doses/concentration levels	0, 1000, 2000, or 4000 mg/kg
Exposure period	3 weeks
Frequency of treatment	5 days/week for 3 weeks
Control Group	Yes
Post exposure observation period	None
Remarks for test conditions	Groups of 3 Charles River CD, COBS male rats were administered 2-nonanone (i.e., methyl heptyl ketone) via gavage, 5 days per week for 3 weeks at doses of 1000, 2000, or 4000 mg/kg bw. Individual body weights and feed consumption were recorded on days 0, 3, 7, 14 and 20 of treatment. All animals were observed daily for clinical signs of toxicity. Necropsy was performed on all test animals, and

	tissues were collected for histological examination.
NOAEL(NOEL)	1000 mg/kg
LOAEL(LOEL)	2000 mg/kg
Actual dose received by dose level and sex	
Toxic response/effects by dose level	
Appropriate statistical evaluations	
Remarks for results	Upon necropsy, no gross compound-related changes were detected at any dose level. Histological examination revealed compound related changes in the stomach and liver at the 2000 and 4000 mg/kg bw/d levels, and in the lungs, kidneys, bladder, adrenal glands, bone marrow, brain, and mesenteric fat at the 4000 mg/kg bw/d level. However, it was not reported whether or not these effects were statistically significant. In the stomach, hyperplasia of the epithelium of the non-glandular mucosa was observed with at varying degrees, which were thought to reflect the amount of contact the test material had with the epithelium and the selection of the tissue specimens for examination. Liver changes were characterized by hepatocyte hypertrophy. In the 4000 mg/kg bw/d group, lungs showed minor acute bronchitis and congestion, edema, and atelectasis; the urinary system had dilatation of the lumena of the renal tubules and multiple hemorrrhages in the bladder (1 rat); the adrenal gland was congested; bone marrow and brains were congested in 2 or 3 rats, respectively; and atrophy of the mesenteric adipose tissue occurred in 1 rat. In the 1000 mg/kg test group, no gross or histopathologic compound-related changes were identified.
Conclusion remarks	The 3-week NOAEL for 2-nonanone in rats is 1000 mg/kg
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Krasavage, W.J., and O'Donoghue, J.L. (1979) Repeated oral administration of five ketones and n-heptane to rats. Unpublished report.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Assay: 72.3 %
Method/guideline	90 day repeat dose study
GLP	No

Year	1980
Species/Strain	Rat/Charles River CD
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	2000mg/kg
Exposure period	90 days
Frequency of treatment	5 days/week
Control Group	Received tap water at a dose of 4000 mg/kg
Post exposure observation period	
Remarks for test conditions	Groups of Charles River CD male rats (8 per group) were administered the test compound undiluted, by gavage 5 days weekly for 90 days. Animals were housed individually and received rodent laboratory chow and tap water ad libitum. Individual body weights and food consumption were determined twice weekly. All animals were observed daily for clinical signs of toxicity. Animals dying during study were autopsied and tissue sample were collected for histopathological evaluation. Prior to termination blood was collected from the posterior vena cava and subjected hematological examination and clinical chemistry determinations. After 90 days surviving animals were sacrificed, and liver, kidney, brain, adrenal glands, testes, heart and spleen weights were measured and relative organ weights were calculated. Tissues were fixed in 10% formalin, embedded in paraffin, stained with hematoxylin/eosin, an examined microscopically. The tissues evaluated include trachea, lung, thymus, heart, tongue, esophagus, stomach, small intestines, large intestines, liver, kidneys, urinary bladder, adrenal glands, pancreas, thyroids, parathyroids, testis, epididymis, spleen, mesenteric lymph nodes, bone marrow, brain (medulla oblongata, cerebellum and cerebral cortex with thalamus and basal ganglia), spinal chord, sciatic-tibia nerves and dorsal root ganglia.
NOAEL(NOEL)	
LOAEL(LOEL)	2000 mg/kg
Actual dose received by dose level and sex	2000mg/kg
Toxic response/effects by dose level	Hind limb weakness was in 1 rat at 59 days and slowly progressed to severe weakness over the next 31 days. Of the seven remaining rats 4 exhibited mild hind limb weakness by 90 days and 2 others showed no hind limb weakness at 90 days. Feed consumption was significantly less for the test group compared to the control group. At 90 days mean body weights were significantly less for the test group. Hematological examination and clinical chemistry determination for the test and control groups revealed normal values. Blood samples collected at 90 days revealed detectable levels of 2-nonanone

	and 2-hexanone. Mean absolute liver, kidney, adrenal gland, and testes weights were greater for test group then for the control group. Mean absolute heart, spleen, and brain were significantly less for the test group compared to the control.
Appropriate statistical evaluations	ANOVA, Bartlett's test and Duncan's multiple range
Remarks for results	The substance was tested at the highest level no causing immediate death. Although 2-nonanone does not possess the structural features to produce any significant amount of a neurotoxic gamma diketone such as 2,5-hexanedione, impurities in commercial grade of 2-nonanone may contain ketones capable of metabolizing to gamma diketones. Therefore, the appearance of "giant axonal swelling" neurotoxicity in treated animals at least 59 days may not be due to the presence of 2-nonanone per se.
Conclusion remarks	Under conditions of the study, a daily oral dose level of 2000 mg/kg bw of a commercial grade of 2-nonanone was inherently toxic to rats inherent.
Data Qualities Reliabilities	Reliability code 3. Not reliable.
Remarks for Data Reliability	Code 3. Does not meet important criteria of current standard methods.
References	O'Donohogue J. L. and Krasavage W. J. (1980) 90-Day repeated oral administration of five ketones and n-heptane to rats. Private communication to FEMA. Unpublished Report.
CAS	4485-09-0
Substance Name	4-Nonanone
Remarks for Substance	Data are for isomer, 2,6-dimethyl-4-heptanone, 67%.
Method/guideline	
GLP	Yes
Year	1980
Species/Strain	Rat/Charles River CD
Sex	Male and Female
Route of administration	Oral-Gavage
Doses/concentration levels	0 and 2000 mg/kg
Exposure period	90 days
Frequency of treatment	Daily
Control Group	Yes
Post exposure observation period	None

Remarks for test conditions	2,6-Dimethyl-4-heptanone (67.0% purity; i.e., diisobutyl ketone) was administered to 8 male Charles River rats by gavage for 90 days at a dose of 0 or 2000 mg/kg bw/day. Following the dosing period, liver, kidney, brain, adrenal glands, testes, heart and spleen weights were recorded and relative organ weights calculated. Hematology and clinical chemistry was performed and results were comparable to controls. At necropsy organ weights were measure and a wide variety of tissues were subjected to histopathological examination.
NOAEL(NOEL)	
LOAEL(LOEL)	2000 mg/kg
Actual dose received by dose level and sex	
Toxic response/effects by dose level	
Appropriate statistical evaluations	
Remarks for results	Absolute and relative liver weights, relative kidney weights, and absolute and relative adrenal gland weights were statistically greater than controls. Absolute but not relative brain and heart weights were significantly depressed. All other organ weights were comparable to controls. No compound related gross pathologic changes were identified. Histopathology examinations were also conducted on the test animals and revealed compound related changes in the stomach, liver, and kidneys. In the stomach, all animals showed hyperkeratosis or hyperkeratosis with pseudoepitheliomatous hyperplasia associated with irritation from direct contact by the solvent. In the liver, minor or moderate hepatocyte hypertrophy was observed. In the kidney, hyaline droplet formation was present in the proximal tubular epithelium suggesting alpha-microglobulin-type neuropathy. There was also a minor occurrence of regenerating tubular epithelium and tubular dilation with casts.
Conclusion remarks	Under conditions of the study, 2000 mg/kg of 2,6-dimethyl-4-heptanone administered by gavage was toxic to both male and female rats.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	O'Donohogue J. L. and Krasavage W. J. (1980) 90-Day repeated oral administration of five ketones and n-heptane to rats. Private communication to FEMA. Unpublished Report.
CAS	821-55-6
Substance Name	5-Nonanone
Remarks for Substance	Assay:98.25%

Method/guideline	90 day repeat dose study
GLP	No
Year	1982
Species/Strain	Rat/Charles River CD
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	233 mg/kg
Exposure period	90 days
Frequency of treatment	5 days/week
Control Group	Received tap water at a dose of 4000 mg/kg
Post exposure observation period	
Remarks for test conditions	Groups of Charles River CD male rats (5 per group) were administered the test compound undiluted, by gavage 5 days weekly for 90 days. Animals were housed individually and received rodent laboratory chow and tap water ad libitum. Individual body weights and food consumption were determined twice weekly. All animals were observed daily for clinical signs of toxicity. Animals dying during study were autopsied and tissue sample were collected for histopathological evaluation. Prior to termination blood was collected from the posterior vena cava and subjected hematological examination and clinical chemistry determinations. After 90 days surviving animals were sacrificed, and liver, kidney, brain, adrenal glands, testes, heart and spleen weights were measured and relative organ weights were calculated. Tissues were fixed in 10% formalin, embedded in paraffin, stained with hematoxylin/eosin, an examined microscopically. The tissues evaluated include trachea, lung, thymus, heart, tongue, esophagus, stomach, small intestines, large intestines, liver, kidneys, urinary bladder, adrenal glands, pancreas, thyroids, parathyroids, testis, epididymis, spleen, mesenteric lymph nodes, bone marrow, brain (medulla oblongata, cerebellum and cerebral cortex with thalamus and basal ganglia), spinal chord, sciatic-tibia nerves and dorsal root ganglia.
NOAEL(NOEL)	233 mg/kg
LOAEL(LOEL)	
Actual dose received by dose level and sex	
Toxic response/effects by dose level	At study termination, both body weights and food consumption were not statistically significant from the control group. Necropsy findings were unremarkable. No giant axonal swelling was observed, although slight neuropathologic changes were observed (myelin ovoid formation, remyelination or adaxonal

	myelin in 3 of 5 rats.
Appropriate statistical evaluations	ANOVA, Bartlett's test and Duncan's multiple range
Remarks for results	The study was designed to screen for ketone neurotoxicity. Dose levels of 1000 mg/kg of 5-nonanone have been shown to produce clear evidence of "giant axonal swelling" neurotoxicity. Doses below 200 mg/kg are not expected to produce any such neurotoxic effects.
Conclusion remarks	Under conditions of the study, a daily oral dose level of 233 mg/kg bw of 5-nonanone was not inherently toxic to rats inherent
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	O'Donohogue J. L. and Krasavage W. J., DiVencenzo G. and Ziegler D.(1982) Commercial grade methyl heptyl ketone (5-methyl-2-octanone) neurotoxicity: Contribution of 5-nonanone.Toxiclogy and Applied Pharmacology, 62, 307-316.
CAS	33083-83-9
Substance Name	5-Undecanone
Remarks for Substance	Data for isomeric ketone, 2,8-dimethyl-5-nonanone. Assay: 99.2 %.
Method/guideline	90 day repeat dose study
GLP	No
Year	1980
Species/Strain	Rat/Charles River CD
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	4000mg/kg
Exposure period	90 days
Frequency of treatment	5 days/week
Control Group	Received tap water at a dose of 4000 mg/kg
Post exposure observation period	
Remarks for test conditions	Groups of Charles River CD male rats (8 per group) were administered the test compound undiluted, by gavage 5 days weekly for 90 days. Animals were housed individually and received rodent laboratory chow and tap water ad libitum. Individual body weights and food consumption were determined

	twice weekly. All animals were observed daily for clinical signs of toxicity. Animals dying during study were autopsied and tissue sample were collected for histopathological evaluation. Prior to termination blood was collected from the posterior vena cava and subjected hematological examination and clinical chemistry determinations. After 90 days surviving animals were sacrificed, and liver, kidney, brain, adrenal glands, testes, heart and spleen weights were measured and relative organ weights were calculated. Tissues were fixed in 10% formalin, embedded in paraffin, stained with hematoxylin/eosin, an examined microscopically. The tissues evaluated include trachea, lung, thymus, heart, tongue, esophagus, stomach, small intestines, large intestines, liver, kidneys, urinary bladder, adrenal glands, pancreas, thyroids, parathyroids, testis, epididymis, spleen, mesenteric lymph nodes, bone marrow, brain (medulla oblongata, cerebellum and cerebral cortex with thalamus and basal ganglia), spinal chord, sciatic-tibia nerves and dorsal root ganglia.
NOAEL(NOEL)	
LOAEL(LOEL)	4000 mg/kg
Actual dose received by dose level and sex	4000 mg/kg
Toxic response/effects by dose level	Two of the 8 animals died by day 3. The test group showed a 17% decrease in food consumption during the first week of treatment. Body weights were also reduced. However, at study termination both body weights and food consumption were not statistically significant from the control group. Blood leukocyte counts were lower for the test group and ASAT and ALT enzyme activities were elevated. The latter changes were not accompanied by any evidence of histopathology. Mean absolute and relative kidney, adrenal, testes, and liver weights were increased for the test group. Histopathological examination revealed hepatocyte hypertrophy and renal hydraline droplet formation, probably the result of alpha-2-microglobulin formation.
Appropriate statistical evaluations	ANOVA, Bartlett's test and Duncan's multiple range
Remarks for results	The substance was tested at or near the acute oral LD50. The study was designed to screen for ketone neurotoxicity.
Conclusion remarks	Under conditions of the study, a daily oral dose level of 4000 mg/kg bw of 2,8-dimethyl-5-nonanone was inherently toxic to rats.
Data Qualities Reliabilities	Reliability code 3. Not reliable.
Remarks for Data Reliability	Code 3. Does not meet important criteria of current standard methods.
References	O'Donohogue J. L. and Krasavage W. J. (1980) 90-Day repeated oral administration of five ketones and n-heptane to rats. Private communication to FEMA. Unpublished Report.

CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexanone derivative, 3,5,5-trimethylcyclohexenone.
Method/guideline	2-yr NTP Bioassay
GLP	Yes
Year	1986
Species/Strain	Rat/Fischer 344/N
Sex	Male and Female
Route of administration	Oral-Gavage
Doses/concentration levels	0, 250, or 500 mg/kg
Exposure period	103 weeks
Frequency of treatment	5 days per week
Control Group	Yes. Received corn oil vehicle only
Post exposure observation period	
Remarks for test conditions	In a two-year study dose levels of 0, 250 or 500 mg/kg bw per day of 3,5,5-trimethylcycloheneone were given to groups of F344/N rats (50/sex/group) by gavage in corn oil 5 days a week daily for 103 weeks (NTP, 1986; Bucher et al., 1986). Food and water were provided ad libitum. Moribund animals were euthanized. Weights were recorded weekly and at the termination of the experiment survivors were sacrificed and necropsies performed.
NOAEL(NOEL)	
LOAEL(LOEL)	250 mg/kg
Actual dose received by dose level and sex	
Toxic response/effects by dose level	Gavage errors accounted for a significant number of deaths (36/300) in both male and female rats. Nephropathy was noted in both test and control rats of both sexes after natural death or at termination. In test animals, increased incidence of mineral deposits in renal collecting ducts (31/50,62% and 20/50, 40%), and tubular cell hyperplasia (1/50, 2% and 4/50, 8%), adenomas (0/50 and 2/50, 8%), and adenocarcinomas (3/50, 6% and 1/50, 2%) were observed in male rats at 250 mg/kg bw per day and 500 mg/kg bw per day, respectively but not in female rats (See Table A3). Tubule mineralization was characterized by basophilic aggregates found in the medullary collecting ducts, often occurring coincidentally with lesions of chronic nephropathy.

Appropriate statistical evaluations	Yes
Remarks for results	
Conclusion remarks	Under conditions of these 2-year gavage studies, there is some evidence of carcinogenicity of 3,5,5-trimethylcycloheneone in the male F344/N rat as shown by the occurrence of renal tubular cell adenomas and adenocarcinomas in animals given 250 or 500 mg/kg/day.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Bucher J.R., Huff J., and Kluwe W.M. (1986) Toxicology and carcinogenesis studies of isophorone in F344 rats and B6C3F1 mice. Toxicology. 39(2), 207-219.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related substance, 2-isopropyl-5-methylcyclohexanol (dl-menthol).
Method/guideline	Carcinogenicity study
GLP	No
Year	1979
Species/Strain	Mouse/B6C3F1
Sex	Male and Female
Route of administration	Oral-Diet
Doses/concentration levels	0, 2,000 or 4,000 ppm (0, 300 or 600 mg/kg bw, respectively)
Exposure period	103 weeks
Frequency of treatment	Daily
Control Group	Basal diet with 2% corn oil
Post exposure observation period	1 week
Remarks for test conditions	A carcinogenicity study was conducted in which groups of 50 B6C3F1 mice of each sex were administered 0, 2,000 or 4,000 ppm dl-2-isopropy-5-methylcyclohexanol in their feed daily for 103 weeks. Dietary concentrations were calculated to provide corresponding average daily intake levels of 0, 300 or 600 mg/kg bw, respectively. Animals were housed five per cage and were observed twice daily for signs of toxicity. Body weights and food consumption were recorded every two weeks for the first twelve weeks, and once a month thereafter. Necropsies and histological examinations were performed on all animals at

	the termination of the study and on those found dead during the study.
NOAEL(NOEL)	300 mg/kg bw/day
LOAEL(LOEL)	600 mg/kg bw/day
Actual dose received by dose level and sex	
Toxic response/effects by dose level	The mean body weights of the male and female mice administered 300 or 600 mg dl-2-isopropy-5-methylcyclohexanol/kg bw were slightly lower when compared to the controls. Survival of the high- and low-dose groups of male mice was similar to the vehicle control animals (controls, 32/50; low-dose, 32/50; high-dose, 35/50). Survival of the high-dose group of female mice was significantly less than that of the control animals (controls, 36/50; high-dose, 45/50). However, decreased survival was not accompanied by any evidence of toxicity in the high-dose group. Survival of the low-dose female mice was similar to the control animals (controls, 36/50; low-dose, 40/50). An increase in the incidence of hepatocellular carcinomas was observed in high-dose male mice (controls, 8/47; low-dose, 8/49; high-dose, 14/48), but was not statistically different from that observed historically in mice of that age and strain [Haseman et al., 1986]. A low incidence of alveolar/bronchiolar adenomas of the lung was observed in both the low- and high-dose females but was not statistically different from the incidence of this neoplasm in historical control groups. Under the conditions of this study, it was concluded that dl-2-isopropy-5-methylcyclohexanol was not carcinogenic and did not produce any organ-specific toxicity for either sex of B6C3F1 mice at dose levels of 300 or 600 mg/kg bw.
Appropriate statistical evaluations	Yes.
Remarks for results	NOAEL based on decreased survival in female mice.
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	National Cancer Institute, NCI (1979) Bioassay of dl-menthol for possible carcinogenicity. U.S. Department of Health, Education and Welfare. National Technical Report Series No. 98.
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexanone derivative 2-Isopropyl-5-methylcyclohexanol.
Method/guideline	Carcinogenicity study

GLP	No
Year	1979
Species/Strain	Rat/F344
Sex	Male and Female
Route of administration	Oral-Diet
Doses/concentration levels	0, 3750, or 7500 ppm (~0, 187 or 375 mg/kg bw, respectively)
Exposure period	103 weeks
Frequency of treatment	Daily
Control Group	Basal diet with 2% corn oil
Post exposure observation period	2 weeks
Remarks for test conditions	Groups of 50 Fischer 344 rats of each sex were administered 0, 3750 or 7500 ppm dl-2-isopropy-5-methylcyclohexanol in their feed daily for 103 weeks. Dietary concentrations were calculated to provide corresponding average daily intake levels of approximately 0, 187 or 375 mg/kg bw, respectively. Animals were housed five per cage until week 48 when the male rats were divided into groups of two to three per cage. The animals were observed twice daily for signs of toxicity. Body weight and food consumption were recorded every two weeks for the first twelve weeks, and once a month thereafter. Necropsies and histological examinations were performed on all animals at the termination of the study and on those found dead during the study.
NOAEL(NOEL)	375 mg/kg bw/day
LOAEL(LOEL)	
Actual dose received by dose level and sex	
Toxic response/effects by dose level	The mean body weights of the male and female rats administered 187 or 375 mg/kg dl-menthol were slightly lower when compared to the controls. Survival of the high- and low-dose groups of male (controls, 31/50; low-dose, 33/50; high-dose, 34/50) and female (controls, 36/50; low-dose, 35/50; high-dose, 38/50) rats was similar to the control animals. Chronic inflammation of the kidney observed in the dosed older males was not considered by the authors to be related to the administration of dl-2-isopropy-5-methylcyclohexanol since the effect is commonly observed in aged male Fischer 344 rats. There was no increase in the incidence of neoplasms of dosed females compared to that of control animals. In the low-dose (10/49) and high-dose (7/49) female groups, fibroadenomas of the mammary glands occurred at a lower incidence than in the control group (20/50). Alveolar/bronchiolar adenomas or carcinomas were reported only for the female control rats. Under the conditions of this study, it was concluded that dl-2-isopropy-5-methylcyclohexanol was neither carcinogenic nor

	toxic for either sex of Fischer 344 rats at dose levels of 187 or 375 mg dl-2-isopropy-5-methylcyclohexanol /kg bw.
Appropriate statistical evaluations	Yes.
Remarks for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	National Cancer Institute, NCI (1979) Bioassay of dl-menthol for possible carcinogenicity. U.S. Department of Health, Education and Welfare. National Technical Report Series No. 98.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexanone derivative 2-Isopropyl-5-methylcyclohexanol.
Method/guideline	90-day toxicity study
GLP	No
Year	1979
Species/Strain	Rat/F344
Sex	Male and Female
Route of administration	Oral-Diet
Doses/concentration levels	0, 930, 1870, 3750, 7500, or 15000 ppm (~0, 93, 187, 375, 750 or 1500 mg dl-2-isopropy-5-methylcyclohexanol/kg bw/day)
Exposure period	13 weeks
Frequency of treatment	Daily
Control Group	Basal diet with 2% corn oil
Post exposure observation period	
Remarks for test conditions	Groups of 10 female and 10 male Fischer 344 rats per group were maintained on diets containing dl-menthol at concentrations of 0, 930, 1870, 3750, 7500, or 15000 ppm for 13 weeks. Dietary concentrations were calculated to provide corresponding average daily intake levels of 0, 93, 187, 375, 750 or 1500 mg dl-2-isopropy-5-methylcyclohexanol/kg bw, respectively. Necropsies were performed on all animals at the end of the study. Histopathological examination was performed on tissues from the control animals, the highest dose group, and selected tissues from the second highest dose group.

NOAEL(NOEL)	750 mg/kg bw/day
LOAEL(LOEL)	1500 mg/kg bw/day
Actual dose received by dose level and sex	
Toxic response/effects by dose level	Final mean body weights of the male and female rats at all dose levels were similar to those of the controls. A slight increase in the incidence of interstitial nephritis was observed in high-dose male rats. No adverse effects were reported for male or female rats administered 93, 187, 375, or 750 mg dl-2-isopropy-5-methylcyclohexanol/kg bw/day.
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	National Cancer Institute, NCI (1979) Bioassay of dl-menthol for possible carcinogenicity. U.S. Department of Health, Education and Welfare. National Technical Report Series No. 98.

CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexanone derivative 2-Isopropyl-5-methylcyclohexanol.
Method/guideline	90-day toxicity study
GLP	No
Year	1979
Species/Strain	Mouse/B6C3F1
Sex	Male and Female
Route of administration	Oral-Diet
Doses/concentration levels	0, 930, 1870, 3750, 7500, or 15000 ppm (~0, 140, 281, 563, 1125 or 2250 mg dl-2-isopropyl-5-methylcyclohexanol/kg bw/day)
Exposure period	13 weeks
Frequency of treatment	Daily
Control Group	Basal diet with 2% corn oil
Post exposure observation	

period	
Remarks for test conditions	Groups of 10 male and 10 female B6C3F1 mice were maintained on diets containing dl-2-isopropyl-5-methylcyclohexanol at dietary concentrations of 0, 930, 1870, 3750, 7500, or 15000 ppm for 13 weeks. Dietary concentrations were calculated to provide average daily intake levels of 0, 140, 281, 563, 1125 or 2250 mg dl-2-isopropyl-5-methylcyclohexanol/kg bw, respectively. Necropsies were performed on all animals at the end of the study. Histopathological examination was performed on tissues from the control animals, the 2250 mg/kg bw/day group, and selected tissues from the 1125 mg/kg bw/day group.
NOAEL(NOEL)	1125 mg/kg bw/day
LOAEL(LOEL)	563 mg/kg bw/day
Actual dose received by dose level and sex	
Toxic response/effects by dose level	Six mice (sex not specified) died during the study but the deaths could not be attributed to compound administration. Final mean body weights of the male mice and female mice were not statistically different from those of the controls except for the high-dose female group which showed statistically significant decreased body weights. A slight increase in the incidence of perivascular lymphoid hyperplasia and interstitial nephritis was reported in the female mice given the two highest dose levels. No adverse effects were reported for male or female mice administered 140, 281 or 563 mg dl-2-isopropy-5-methylcyclohexanol/kg bw/day.
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	National Cancer Institute, NCI (1979) Bioassay of dl-menthol for possible carcinogenicity. U.S. Department of Health, Education and Welfare. National Technical Report Series No. 98.
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for mixture of structurally related alkyl-substituted cyclohexanones and cyclohexanols: 1)46.8% (1a, 2ß, 5a)-2-isopropy-5-methylcyclohexanol 2)3.97% (1a, 2a, 5a)-2-isopropy-5-methylcyclohexanol 3)0.86% (1 ß, 2ß, 5a)-2-isopropy-5-methylcyclohex

Method/guideline	28-Day Oral Toxicity Study
GLP	Yes
Year	1990
Species/Strain	Rat/Sprague Dawley
Sex	Male and Female
Route of administration	Oral Gavage
Doses/concentration levels	0, 100, 200, or 400 mg/kg bw
Exposure period	29 or 30
Frequency of treatment	Once daily
Control Group	Yes, vehicle only
Post exposure observation period	
Remarks for test conditions	Groups (10/sex/group) of male and female Sprague-Dawley rats were given daily dose levels of 0, 100, 200, or 400 mg/kg bw of a mixture of alkyl-substituted cyclohexanol by gavage in corn oil (10 ml/kg) daily for 29 or 30 days. Clinical signs were monitored twice weekly and body weights and food consumption were measured weekly. At the initiation of the study, 10 animals were randomly selected from the pool of animals not selected fro the study. They were fasted overnight and blood samples were drawn and analyzed for baseline clinical chemistry and hematology parameters. Prior to termination, animals were injected with ketamine and blood samples were drawn for clinical chemistry and hematology. At necropsy, organ weights (brain, spleen, liver, heart, kidneys, testes with epididymides, adrenals, ovaries, and pituitary) were measured, and tissues (26) were preserved in 10% formalin. All tissues from the control and high-dose groups and tissues from the heart, liver, kidneys, and gross lesions from the low- and mid-dose group were embedded in paraffin, stained with hematoxylin and eosin, and examined microscopically.
NOAEL(NOEL)	Less than 100 mg/kg bw per day for males and 400 mg/kg bw per day for females.
LOAEL(LOEL)	100 mg/kg bw per day (based on appearance of alpha-2-microglobulin effect in males).
Actual dose received by dose level and sex	0, 100, 200, or 400 mg/kg bw
Toxic response/effects by dose level	All animals survived to study termination with high dose males showing increased incidence of urine staining during clinical observations. Except for a non-statistically significant decrease in mean body weigh in high-dose males, there were no statistically significant differences in body weight or food consumption between treated and control groups. A significant decrease in serum glucose levels was reported in the mid- and high-dose males that the authors, in part, attribute to change in nutritional status as revealed by a decreased body weights in

	the high-dose group. A treatment-related increase in alkaline phosphatase was reported in high-dose males. Measurement of body weight, food consumption, hematology and clinical chemistry parameters revealed no significant changes between test and control female rats. There were statistically significant increases in relative kidney weights in high-dose males. Histopathological findings revealed renal tubule protein droplets in all groups of treated male rats. The authors considered these findings related to the lysosomal handling of alpa-2-micro-globulin, a protein specific to the male Sprague-Dawley rat. Absolute and relative liver weights in high-dose females also were significantly increased but these changes were not confirmed by histopathological examination.
Appropriate statistical evaluations	Dunnett's Control versus Treatment Comparison.
Remarks for results	Based exclusively on the renal pathology (alpha-2-microglobulin effect) reported in all dosed groups of male rats, the authors concluded that the no observable adverse effect level (NOAEL) for the mixture is less than 100 mg/kg bw per day in male rats and 400 mg/kg bw per day in female rats.
Conclusion remarks	The NOAEL is less than 100 mg/kg bw in male Sprague-Dawley rats and 400 mg/kg bw per day for female rats.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Serota D. G. (1990) 28-Day oral toxicity study in rats: B100. HLA Study No. 642-477. Private Communication to FEMA. Unpublished Report.
CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for structurally related substance 2-hexanone, 5-methyl-, and purity 99.2%.
Method/guideline	
GLP	No
Year	1979
Species/Strain	Rat/Charles River CD
Sex	Male
Route of administration	Oral-Gavage
Doses/concentration levels	0 and 2000 mg/kg
Exposure period	90days

Frequency of treatment	A single daily gavage 5 days/week
Control Group	Yes; treatment with water
Post exposure observation period	None
Remarks for test conditions	This study involved only a single maximum tolerated dose, and was designed to determine the neurotoxicity and subchronic effects of a series of different ketones against that of n-heptane. Body weight and feed consumption was assessed twice weekly. A full complement of tissues was harvested for histopathology with special emphasis placed on the handling and collection of neural tissues. Several tissues were also weighted. Complete hematology and clinical chemistries were also conducted.
NOAEL(NOEL)	Not established.
LOAEL(LOEL)	
Actual dose received by dose level and sex	
Toxic response/effects by dose level	
Appropriate statistical evaluations	Yes, one-way ANOVA
Remarks for results	No evidence of neurotoxicity was seen based on an absence of alterations in appearance or behavior, and histological changes in nervous tissue. Feed intake was, in general, slightly depressed throughout the study and was significantly lower during the first week. Body weights were significantly reduced at essentially all time points. There was no effect on the erythron. Effects noted in the clinical chemistry profile included slight, but statistically significant, increases in SGOT, SGPT and urea nitrogen. Urea nitrogen levels were still within levels seen in historical controls. Absolute and relative increases in liver and adrenal weights were seen. Relative increases were seen in other tissues; however, their significance is negated by a significantly decreased bodyweight. Histological evidence of gastric irritation was manifested by hyperkeratosis, and hyperkeratosis with pseudoepitheliomatuos hyperplasia and submucosal thickening and edema. Liver changes consisted of a diffuse hepatocyte hypertrophy, and microfoci of hyperplasia in some rats. The latter effect was characterized by an increase in cytoplasmic and generally nuclear size. Three types of nodules were present. The first type was identified on the basis of diffuse increase in cytoplamic masophilia, the second type contained heavily vacuolated cells, and the third had very large vesicular nuclei with prominent nucleoli. These types of nodules are generally regarded as pre-neoplastic changes. A few animals also exhibited necrosis of individual hepatocytres, a few others had vacuolation of individual hepatocytes. Some animals also had bile duct epithelial hyperplasia. Renal changes included and increased incidence of regenerating tubular epithelium and dilatation with casts, and hyaline droplet

	formation in the proximal tubular epithelium.
Conclusion remarks	Other than the finding of a diffuse hepatocyte hypertrophy, the observation of microfoci of hyperplasia was not reproduced following inhalation exposure. Inhalation is the most relevant route by which humans are exposed. Peak blood levels at the highest exposure level in the inhalation study were similar to that following oral intubation.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 1. Comparable to guideline study.
References	Eastman Kodak Co. (1979) 90-day repeated oral administration of five ketones and n-heptane to rats. Unpublished report.
CAS	2345-28-0 2
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related cyclohexanone derivative 2-Isopropyl-5-methylcyclohexanol.
Method/guideline	14-day minimum toxicity screen
GLP	Yes
Year	1987
Species/Strain	Rat/Fischer 344
Sex	Male and Female
Route of administration	Oral-Diet
Doses/concentration levels	10 mg/kg bw/day
Exposure period	14 days
Frequency of treatment	Continuously in the diet
Control Group	Basal diet
Post exposure observation period	
Remarks for test conditions	Groups of 5 male and female Fischer 344 rats were maintained on a diet containing 2-pentadecanone in corn oil at levels calculated to provide an average daily intake of 10 mg/kg bw. Control groups received the basal diet and the corn oil vehicle only. Body weight and food consumption were measured weekly. At necropsy on day 14, liver and kidneys were weighed and prepared for histopathology.
NOAEL(NOEL)	10 mg/kg bw/day
LOAEL(LOEL)	
Actual dose received by	

dose level and sex	
Toxic response/effects by dose level	No effects were reported
Appropriate statistical evaluations	
Remarks for results	The 14-day NOEL for the administration of 2-pentadecanone in the diet was reported to be 10 mg/kg bw.
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basis data given. Comparable to guideline study.
References	Van Miller J.P. and Gill M. W. (1987) 14-day dietary minimum toxicity screen of 4-(2-furyl)-3-buten-2-one, oxotetradecanoic acid glyceride, 3-oxooctanoic acid glyceride, 2-pentadecanone, and o-methoxybenzaldehyde. Unpublished report to FEMA

4.4 Reproductive Toxicity

CAS	123-18-2
Substance Name	2,6,8-Trimethyl-4-nonanone
Remarks for Substance	Assay: >91%
Method/guideline	OECD Guideline No. 422, A Combined Repeated Dose Toxicity Study with the Reproduction/Developmental Toxicity Screening Test. U.S. EPA OPPTS 870.3650, Combined repeated dose toxicity study with the reproduction/developmental toxicity screening test
Test Type	
GLP	Yes
Year	2002
Species/Strain	Rat/CD
Sex	Male/Female
Route of administration	Oral-Gavage
Duration of test	males 10 days post-mating; females lactation day 4.
Doses/concentration levels	100, 300 and 1000 mg IBHK/kg/day
Premating Exposure period for males	Males- 2 weeks prebreeding, two weeks breeding and 10 days post-breeding. Females- 2 weeks prebreeding, two weeks

	breeding, through gestation (3 weeks) and lactation (4 days)
Premating Exposure period for females	2 weeks
Frequency of treatment	Daily
Control Group and treatment	Yes, vehicle only
Remarks for test conditions	Male and female CD rats (12/sex/group), age 8 weeks of age were given daily doses of 0, 100, 300, or 1000mg/kg of IBHK by gavage in a corn oil suspension for 2 weeks prebreeding, two weeks breeding, and 10 days postbreeding for males and 2 weeks prebreeding, two weeks breeding, through gestation (3 weeks) and lactations (4 days). Samples were analyzed to confirm homogeneity, stability and concentration verification. Parameters monitored during the study included: -Clinical observations performed and frequency; Clinical observations were conducted daily throughout the study period. -Detailed Clinical Observations (DCO): Conducted on all rats before-exposure and weekly throughout the study. Mated females received DCO examinations on gestation day (gd) 0, 7, 14 and 20, and lactation day (Id) 4. The DCOs included cage-side, hand-held and open-field observations that were recorded categorically or using explicitly defined scales. -Functional Tests: The functional tests included a sensory evaluation (nociception and startle response), rectal temperature, grip performance and motor activity. -Body weight/body weight gain: All rats were weighed at least once in the pre-exposure period. Male body weights were recorded weekly throughout the study. Female body weights were performed weekly for the premating and mating periods. Maternal body weights were recorded on GD 0, 7, 14, 17 and 20. Females that delivered were weighed on Id 1 and 4. Females that failed to mate or deliver were weighed on a weekly basis for the study duration. -Food consumption: Food consumption was determined weekly for males and females during the pre-mating period. Due to co-housing, food consumption was not measured during mating. Following breeding, food consumption was not measured for the males. During gestation, food consumption for the females was measured on gd 0, 7, 14, 17 and 20. After parturition, food consumption was measured on Id 1 and 4. Food consumption was not recorded for females that did not mate or deliver. -Breeding Procedures: During the 2 week mating period, one male and one female from the same dose group were co-habitated until pregnancy occurs or the mating period is over. Females were examined daily for a vaginal copulatory plug or the vaginal presence of sperm determined by vaginal lavage samples. If pregnancy was not determined by the end of the mating period, the animals were separated and housed individually for the remainder of the study. -Litter Data: Females were observed for signs of parturition beginning on gd 20. The first day the presence of a litter was noted was designated Id 0. All litters were examined as soon as

possible after delivery and the following information was recorded: date of parturition, litter size on gd 0, the number of live and dead pups on gd 0, 1 and 4 post-partum and the sex and weight of each pup on postnatal day (pnd) 1 and 4. Pup clinical observations were recorded on pnd 0, 1 and 4. In addition, any physical abnormalities or demeanor changes were recorded during the lactation period. Any pups found dead were sexed, examined grossly for external and visual effects, if possible and discarded

Clinical Pathology: On the day prior to necropsy, all animals were fasted overnight. At necropsy, animals were anesthetized with carbon dioxide and blood samples were removed from the orbital sinus. Blood samples were not taken from females that failed to deliver a litter.

-Hematology Assays: hematocrit (HCT), hemoglobin concentration (HgB), red blood cell (RBC) count, total white blood cell (WBC) count, platelet (PLAT) count, differential WBC count, and red blood cell indices including mean corpuscular hemoglobin (MCH), mean corpuscular volume (MCV), and mean corpuscular hemoglobin concentration (MCHC).

-Coagulation Assay: prothrombin time (PT).

-Clinical Chemistry Assays: Enzyme activities of alkaline phosphatase (AP), alanine aminotransferase (ALT), and aspartate aminotransferase (AST), and concentrations of: albumin (ALB), cholesterol (CHOL), creatinine (CREAT), electrolytes (Na, K, PO4, CI and Ca), glucose (GLU), total bilirubin (TBIL), total protein (TP), and urea nitrogen (UN).

Urine was collected from all male rates in each dose group during the week prior to necropsy. Animals were housed overnight in metabolic cages.

-Urinalysis Assays: Color, appearance, specific gravity, and urine volume. Semiquantitative analysis: pH, bilirubin, glucose, proteins, ketones, blood, and urobilinogen.

-Anatomic Pathology: A complete necropsy of all animals was performed. Male rats were necropsied on study day 39. Females that delivered were necropsied on Id 5. Female rats that did not deliver were necropsied at least 24 days after the last day of the mating period. The necropsy included an examination of: the external tissues and all orifices, the cranial, nasal, thoracic and abdominal cavities, and all viscera. Selected tissues of the viscera were incised. Examination of uterus: An examination of the uterus for the number of implantation sites was recorded. The uteri of females that did not deliver were stained to determine pregnancy status.

-Organ weights: The following organs were trimmed and weighed: testes, epididymides, seminal vesicles with coagulating glands (and seminal fluid), prostrate, ovaries, liver, kidneys, adrenals, thymus, spleen, brain, thyroid/parathyroid (after fixation) and heart.

-Histopathology: Histological examinations were conducted on numerous tissues, including tissues exhibiting gross lesions, from all adult rats in the control and high-dose groups, as well

as any rats found dead or sacrificed moribund. The histopathological examination of the testes included a qualitative assessment of the stages of spermatogenesis. Microscopic evaluation involved a qualitative assessment of the relationships between spermatogonia, spermatocytes, spermatids and spermatozoa in the seminiferous tubules. Sections of the testes were also examined for the presence of degenerative changes. Also, the liver (males and females), kidneys (males), thyroid glands (males) and gross lesions (males and females) were examined at all dose levels as significant findings were present between the control and high-dose group

NOAEL(NOEL)

A no-observed effect level (NOEL) for general toxicity could not be determined for male rats due to the sex-specific incidence of alpha-u-nephopathy, while the NOAEL for general toxicity in females was 100 mg/kg/day. The NOEL for reproductive effects was 300 mg/kg/day. The NOEL for neurological effects was 1000 mg/kg/day, the highest dose level tested

LOAEL(LOEL)

Female NOAEL=100 mg/kg bw: Reproductive NOAEL=300 mg/kg bw

Actual dose received by dose level and sex

0, 100, 300, or 1,000 mg/kg bw

Parental data and F1 as appropriate

Mortality and day of death: none

-In-Life Observations: Oral administration of IBHK resulted in increased salivation (padoral staining - clear) at all dose levels in both sexes. Salivation was transient, usually ending within one hour of dosing, suggesting a local response to the taste of the test material. Perineal urine soiling was increased in males in the 1000 mg IBHK/kg/day group.

Salient Male Clinical Observations

Male Clin Obs

Dose Level (mg/kg/day) # Animals Affected)

	0	100	300	1000
Males				
Perioral Soiling - Clear	1	7*	11 *	12"
Perineal Soiling - Urine	0	0	0	4*
Females				
Perioral Soiling - Clear	2	8*	12 *	12"

• Indicates effects considered to be treatment-related.

Clinical examinations performed on all rats revealed no treatment-related or statistically significant findings in the treatment groups as compared to the control group in either sex.

Body weight/body weight gainshowed no significant differences in body weight or weight gain were observed for males at any test level during the 6 weeks of exposure. There were also no treatment-related significant differences in the body weights or body weight gains of females at any dose level tested during

the pre-mating, gestation or lactation periods.

There were no significant differences in feed consumption between control and test animals in either sex.

Reproductive Indices including pup survival and sex ratio were monitored. There were no treatment-related effects at any dose level on any of the reproductive parameters, pup survival indices or sex ratio that were evaluated. Pup survival was significantly higher than controls on Id 1 in the 300 and 1000 mg/kg/day dose groups; however, this finding is attributed to the lower value in the control group and was not considered adverse. There was a small, statistically significant decrease in gestation length of the 100 and 1000 mg/kg/day dose groups. However the value was within the range of the historical control data and not considered to be treatment-related.

Litter observations recorded in the offspring occurred at low frequency and bore no relationship to treatment. One low-dose pup was observed with hindllmb rotation, but this was an isolated occurrence bearing no relationship to treatment. Litter size and pup body weights showed decreases in pup body weights of male and female pups on pnd day 1 and 4 in the 1000 mg/kg/day dose group were initially identified as being statistically different from controls using an ANOVA, however, due to the increased litter size in the high-dose group, an ANCOVA was used to determine if the difference in pup body weight was due to litter size and not treatment. The ANCOVA indicated that the effects on pup body weight were not significant on pnd 1 but were significant on pnd 4

Significant Effects on Mean Pup Weights

Mean Pup Weights	Dose Level (mg/kg/day)			
Parameter (mean) Values	0	100	300	1000
1Female (g)	7.0	6.5	6.5	6.1a
1Male (g)	7.4	6.9	6.8	6.4a"
4 Female (g)	10.1	9.1	9.1	8.3a*
4 Male (g)	10.7	9.5	9.5	8.5a*

a = indicates effects considered to be treatment related.

* Statistically different from control mean by Dunnett's test, alpha=0.05

Sensory evaluation of males and females at termination revealed no treatment-related findings. Treatment did not affect the rectal temperature of either sex. There were no treatment-related effects on the hindlimb or forelimb grip performance in either male or female rats.

Treatment did not affect total motor activity count in either sex. The distribution of the motor activity counts within a session were also not affected by treatment in males, however, was statistically different for the females. For interpretation of this statistically significant tdple interaction, additional examination

of the data was performed. All of the double interactions containing treatment, time or epoch were examined, indicating that there was a significant difference in time-epoch, but that it was due to a difference in days not treatment. The female data for overall count distributions for the four treatment groups displayed differences from baseline and post-treatment conditions, irrespective of treatment. Linear contrasts indicated that that triple interactions were not statistically significant and the p values do not support a dose-response relationship. The interpretation of these data led to the conclusion that the statistically significant triple interaction in female rats represents a difference between days rather than an effect of treatment.

Haematology revealed that males given 300 or 1000 mg/kg/day had haemoglobin levels that were slightly lower (statistically significant) than the controls. The differences were not considered treatment-related as they were within, or in close proximity to, the historical control range.

The prothrombin time for males in the 1000 mg/kg/day dose group was higher than controls, statistically significant and outside of the historical control range.

Salient Coagulation Findings

Sex	Males			
Dose (mg/kg/day)	0	100	300	1000
Prothrombin time (sec)	13.1	13.2	13.7	15.8a*

A = indicates effects judged to be treatment-related.

*Statistically significant from control mean by Dunnett's test, alpha=0.05

Clinical chemistry determinations revealed serum cholesterol levels in males and females in the 1000 mg/kg/day group were statistically higher than the control and slightly outside of the historical control range. The differences were considered to possibly be treatment-related, but not toxicologically significant because increase compared to the historical control data (43-58 mg/dl for males and 42-73 mg/dl for females) was minor. The AST and total protein of males in the 1000 mg/kg/day group were higher and lower, respectively, than the control values and statistically identified. Alterations in AST were considered treatment-related, but secondary to the hepatocellular hypertrophy noted in the necropsy of these animals. ALP activity in the 1000 mg/kg/day females was lower than the control and historic values (66-97 u/l). While this was considered treatment related, it was not considered toxicologically significant due to the minor nature of the difference and lack of apparent adverse effects. The urea nitrogen values of males in the 300 and 1000 mg/kg/day groups was marginally higher than that of control; however, the differences were minor, within the historic range (13-14 mg/dl) and not considered treatment-related. Females given 100 mg/kg/day had significantly lower albumin than controls, but this was not considered treatment-related as the higher dose groups did not display similar responses.

Salient Clinical Chemistry Findings

Sex	Males				Females			
Dose (mg/kg/day)	0	100	300	1000	0	100	300	1000
CHOL (mg/dl)	42	45	48	61a*	53	52	63	74a*
AST (u/l)	97	86	83	77a*	108	90	107	98
Total Protein (g/dl)	6.5	6.5	6.5	7.0a*	6.5	6.3	6.6	6.7
Albumin (g/dl)	3.4	3.3	3.3	3.5	3.4	3.3*	3.4	3.5
ALP(u/l)	142	132	158	127	91	84	100	64a**
Urea Nitrogen (mg/dl)	14	14	16"	15"	17	19	18	18

* Statistically significant from control mean by Dunnett's test, alpha=0.05.

** Statistically significant from control mean by Wilcoxon's test, alpha=0.05.

a = indicates the effects judged to be treatment-related.

The urine pH of males in the 1000 mg/kg/day dose group was more acidic than the controls and the ketone levels were slightly lower than the control levels. These differences were outside the historical control range and considered to be to be treatment-related. A few males in the 300 mg/kg/day group also had slightly more acidic urine pH. This acidic urine pH could be secondary to the degenerative changes in the kidneys of the males, but could also be associated with the acidic metabolites of IBHK.

Dose-related increases in absolute and relative liver weights occurred in males and females given 100, 300 or 1000 mg/kg/day. Absolute and/or relative kidney weights of males and females given 300 or 1000 mg/kg/day were also increased. These differences were statistically identified and outside of the historical control data. Therefore, the differences were considered to be treatment-related.

Absolute and/or relative thyroid weights of males given 100 or 1000 mg/kg/day and females given 300 or 1000 mg/kg/day were higher than control weights and were statistically identified, higher than historical control data and considered to be treatment-related. The relative weight of the ovaries of the females given 100 mg/kg/day was significantly increased as compared to controls and increased as compared to the historical data. However, this difference was not considered to be treatment-related given the normal reproductive performance of these females, lack of any histological changes, and the minor difference from controls. In addition, the absolute and relative ovarian weights from all dose levels in this study, including controls, were lower than historical controls.

Salient Organ Weights

Sex	Males			
Dose (mg/kg/day)	0	100	300	1000
Terminal Body (g)	390.5	400.3	394.1	385.9
Liver (g)	11.269	13.044a*	14.005a*	17.678a*
Liver (g/100)	2.871	3.262a*	3.557a*	4.581 a*
Kidney (g)	2.868	3.035	3.591a*	4.222a*
Kidney (g/100)	0.736	0.758	0.912a**	1.096a**
Thyroid (g)	0.0164	0.0193"	0.0186	0.0222a*
Thyroid (g/100)	0.0042	0.0048	0.0047	0.0058a*

* Statistically significant from control mean by Dunnett's test, alpha=O.05. ** Statistically significant from control mean by Wilcoxon's test, alpha=0.05.

a = indicates the effects judged to be treatment-related.

g/100 = organ weight per 100 grams of body weight

Sex	Females			
Dose (mg/kg/day)	0	100	300	1000
Terminal Body (g)	272.0	273.2	273.2	259.8
Liver (g)	9.810	10.802a*	12.077a*	14.167a*
Liver (g/100)	3.612	3.944a*	4.417a*	5.445a*
Kidney (g)	1.934	1.992	2.110	2.121
Kidney (g/l00)	0.712	0.726	0.770a*	0.817a*
Thyroid (g)	0.0143	0.0162	0.0177a*	0.0196a*
Thyroid (g/lO0)	0.0053	0.0059	0.0065a*	0.0076a*
Ovaries (g)	0.113	0.126	0.126	0.128"
Ovaries (g/100)	0.042	0.046	0.046	0.049"

* Statistically significant from control mean by Dunnett's test, alpha=0.05. ** Statistically significant from control mean by Wilcoxon's test, alpha=O.05. a = indicates the effects judged to be treatment-related. g/100 = organ weight per 100 grams of body weight

There were no treatment-related gross pathologic observations.-Histopathology examinations revealed male rats given 100, 300 or 1000 mg/kg/day had degenerative kidney effects that were in excess of that observed in the control male rats and were interpreted to be treatment related. Male rats given 1000 mg/kg/day had degenerative changes involving the renal tubules that were slight to moderate in severity compared with controls. This lesion primarily involved the proximal convoluted tubules and was characterized by an increase in cytoplasmic basophilia of tubular epithelial cells, thickening of

the tubular basement membrane, presence of granular casts within the tubular lumens and the interstitial accumulation of mononuclear inflammatory cells. Necrotic tubular epithelial cells were also noted in the majority of males given the 1000 mg/kg/day were multifocal in distribution and very slight in severity. Male rats given 300 mg/kg/day had similar degenerative tubular changes of slight to moderate severity, and some of these rats had a very slight necrosis of tubular epithelial cells. Male rats given 0 or 100 rng/kg/day had a very slight tubular degeneration that was similar to the degeneration seen in the males of the higher dose groups. This slight degeneration occurred in 3 of 12 control males as compared to 7 of 12 males given 100 mg/kg/day. The increased incidence of this observation in males given 100 mg/kg/day was considered to be treatment-related. Degenerative kidney lesions were noted in females given 0 or 1000 mg/kg/day but were interpreted to be spontaneously occurring because of the low incidence and minimal severity.

Male rats given 100, 300 or 1000 mg/kg/day also had eosinophilic staining (hyalin) cytoplasmic inclusions/droplets in the proximal tubules, which were infrequently observed in the control males, not observed in any of the females and was interpreted to be treatment-related. The results were consistent with, but not diagnostic for, alpha 2u globulin accumulation. Increased levels of this protein in the proximal convoluted tubular cells of male rats has been shown to cause tubular degeneration, although this is not considered relevant for human risk assessment as humans do not develop nephropathy due to differences in this protein.

Males given >/= 100 mg/kg/day and females given >/= 300 mg/kg/day had treatment-related hypertrophy of hepatocytes in the liver. The effect was more prominent in males, given that it was seen even at the lowest dose point and based on the panlobular distribution within the hepatic Iobule. Males given *>/=100* mg/kg/day had treatment-related hypertrophy of follicular epithelial cells of the thyroid gland. Thyroid effects were not observed in female rats.

Offspring toxicity F1 and F2 .

Appropriate statistical evaluations

Yes. Descriptive statistics (means and standard deviations) were reported for RBC indices and WBC differential counts. Parental body weights, gestation and lactation body weight gains, litter mean body weights, feed consumption, urine volume, urine specific gravity, coagulation, clinical chemistry data, appropriate hematologic data and organ weights (absolute and relative) were first evaluated by Bartlett's Test for equality of variances. Based on the outcome, a parametric or nonparametric test analysis of variance (ANOVA) was performed. If the ANOVA was significant (alpha=0.05), then a Dunnett's Test or the Wilcoxon Rank-Sum Test with Bonferroni's correction was performed. The mean pup body

	weights for postnatal day (pod) 1 and 4 were analyzed with an analysis of covariance (ANCOVA), where the covariate was litter size on pnd 1 and 4 respectively. The ANCOVA was run first with the interaction between dose and the covariate included. If the interaction was not significant, the analysis was run again without the interaction. If the dose effect was significant at alpha=0.05 in the second run, the least square means were calculated and the dosed groups were compared to the control groups by a t-test. The gestation length, average time to mating and litter size were examined with a non-parametric ANOVA. If there was significance, the Wilcoxon Rank Sum Test with Bonferroni's correction was performed. Statistical outliers were identified by a sequential method and were only excluded from the analysis for documented, scientifically sound masons. The mating, conception, fertility and gestation indices were analyzed by the Fisher exact probability test with Bonferroni's correction. Evaluation of the neonatal sex ratio on lactation day (ld) 1 was performed by the binomial distribution test. Survival indices, post-implantation loss and other incidence data among neonates were analyzed using the litter as the experimental unit by the censored Wilcoxon test as modified by Haseman and Hoel with Bonferroni's correction. DCO and sensory evaluation incidence scores were statistically analyzed by a z-test of proportions comparing each treated group to the control. Data collected at each time point were analyzed separately. Rectal temperature and grip performance were analyzed by ANCOVA with exposure as the factor and the covariate of the pre-exposure time point measure of the variable. The first examination of the ANCOVA was for the treatment by pre-exposure measure interaction and if this was significant, then an ANVOA was run separately for each time point. If the dose effect was significant, the least square means were generated and a t-test performed. Motor activity counts were reported as their square roots and analyzed by a repeated-measure design with treatment as the factor and the repeated factor of time. Motor activity also had the repeated factor of epoch (within time) in the model. The inclusion of pre-exposure data in the analysis made relevant only the analyses that included factors of both treatment and time. The primary interactions examined were treatment-by-time and treatment-by-time-by-epoch. Linear contrasts were calculated to determine which treatment groups differed from the control if either of these interactions were significant. The probability values were reported without correction
Remarks for results	
Conclusion remarks	A no-observed effect level (NOEL) for general toxicity could not be determined for male rats, while the NOAEL for general toxicity in females was 100 mg/kg/day. The NOEL for reproductive effects was 300 mg/kg/day. The NOEL for neurological effects was 1000 mg/kg/day, the highest dose level tested
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.

References	Dow Chemical (2002) OECD Guideline No. 422, A Combined repeated dose toxicity study with the reproduction/ developmental toxicity screening test with 2,6,8-trimethyl-4-nonanone. Unpublished Report.
CAS	823-55-2
Substance Name	2,4-Dimethylcyclohexanone
Remarks for Substance	Data are for mixture of structurally related alkyl-substituted cyclohexanones and cyclohexanols. 1) 46.8% (1a, 2ß, 5a)-2-isopropy-5-methylcyclohexanol 2) 3.97% (1a, 2a, 5a)-2-isopropy-5-methylcyclohexanol 3) 0.86% (1 ß, 2ß, 5a)-2-isopropy-5-methylcyclo
Method/guideline	in vivo Reproductive and Developmental Toxicity Screening Test
Test Type	
GLP	Yes
Year	1989
Species/Strain	Rat/Sprague Dawley
Sex	Female
Route of administration	Oral-Gavage
Duration of test	39 days
Doses/concentration levels	0, 150, 750, or 1,500 mg/kg bw
Premating Exposure period for males	
Premating Exposure period for females	7 days
Frequency of treatment	Daily
Control Group and treatment	Yes, vehicle only (corn oil)
Remarks for test conditions	Groups of ten female rats were orally administered an oil containing a mixture of alkyl-substituted cyclohexanone derivatives via gavage at dose levels of 0, 150, 750 or 1500 mg/kg bw/d for seven days prior to and through cohabitation, gestation, delivery and a four day lactation period. The vehicle was corn oil. Body weights, food consumption and clinical signs were recorded throughout the observation period. All dams were necropsied and examined for gross lesions on Day 25 of presumed gestation for rats not delivering a litter and four days postpartum for rats delivering a litter. Pups delivered were sacrificed on day 4 post partum; any pups dying during the lactation period were necropsied.
NOAEL(NOEL)	150 mg/kg bw

LOAEL(LOEL)

Actual dose received by dose level and sex	0, 150, 750, or 1,500 mg/kg bw
Parental data and F1 as appropriate	Deaths or moribund sacrifice were reported in 2/10 females at 750 mg/kg bw per day and 5/10 females at 1,500 mg/kg bw per day. Additional clinical observations included decreased motor activity, ataxia, dysnea, rales, chromorrhinorrhea, un-groomed coat and thin appearance at the 750 and 1500mg/kg bw per day dose levels. Urine stained fur and excess salivation were observed at all dose levels. Significant (P < or = 0.05) decreases in body weight and food consumption were reported during the pre-mating period in the 750 and 1500 mg/kg bw per day groups compared to those for control group. A non-statistically significant decrease in maternal body weight gain was reported in the 750 mg/kg bw per day group compared to the control group. The single dam that delivered a litter in the high-dose group also showed less weight gain. Absolute and relative feed consumption were comparable between the low-, mid, and control groups. On day 1 of lactation, the average body weight of dams in the mid-dose group and the single dam in the high-dose group was significantly (P < or =0.01) less than in the control group. During lactation, dams in the mid-dose group gained weight while the weight gain in the single dam in the high-dose group were comparable to that for the control group. Compared to control animals, feed consumption in the mid- and high-dose group decreased significantly (P< or =0.01) during premating but was increased significantly (P< or =0.01 to 0.05) during lactation. Of the rats surviving the cohabitation period 4 of 5 became pregnant at the highest dose level (1500 mg/kg bw per day). Live litters were reported for 9/19, 8/10, 5/6, and 1/4 pregnant females in the control, 150, 750, and 1500 mg/kg bw per day groups, respectively. Increased number of dams with stillborn pups, stillborn pups, and late resorptions in utero were reported in the 750 mg/kg bw per day group. At 1500 mg/kg bw per day, 2 rats had only resorptions in utero when found dead on gestation day 23 and one rat possessed only empty implantation sites in utero on day 25 of presumed gestation.
Offspring toxicity F1 and F2	On day 1 postparturition, litters of dams in the 750 and 1500 mg/kg bw per day groups showed non-statistically significant decreases in pup weight which by day 4 were comparable to controls in the mid-dose group, but less than the control value in the high dose group. On day 4 postpaturition, significant (P< or = 0.01) increases in pup mortality were reported in the mid- and high-dose groups compared to controls. However, even at the highest dose level, there was no evidence of an effect of the test article on implantation, duration of gestation, pup sex ratio, or gross morphology of pups.

Appropriate statistical evaluations	Yes
Remarks for results	
Conclusion remarks	Authors concluded that the maternal no adverse effect level (NOAEL) for reproductive effects was 150 mg/kg bw per day and the offspring NOAEL for developmental effects is higher than 150 mg/kg bw per day, but less than 750 mg/kg bw per day.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Comparable to guideline study with acceptable restrictions.
References	Hoberman A. M. (1989) Reproductive and developmental toxicity screening of B100 administered orally via gavage to Crl:CD(SD)Br female rats. Argus Research Laboratories, Inc. Protocol 412-015. Private Communication to FEMA. Unpublished Report.
CAS	823-55-2
Substance Name	2,4-Dimethylcyclohexanone
Remarks for Substance	Data are for alkyl-substituted cyclohexanol, 2-Isopropyl-5-methylcyclohexanol
Method/guideline	
Test Type	Dominant lethal assay-Acute study
GLP	No
Year	1975
Species/Strain	Random bred rat
Sex	Male
Route of administration	Oral-Gavage
Duration of test	
Doses/concentration levels	Test 1: 1.45, 14.5, or 145 mg/kg bw; test 2: 500 or 3000 mg/kg bw
Premating Exposure period for males	
Premating Exposure period for females	
Frequency of treatment	Single dose
Control Group and treatment	Saline
Remarks for test conditions	Groups of male rats were gavaged with 1.45, 14.5 or 145 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 1) or 500 or 3000 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 2). Male rats

	were mated with 2 female rats per week for 8 weeks. 14 days after mating, females were killed and the uterus was examined for early deaths, late fetal deaths and total implantations.
NOAEL(NOEL)	
LOAEL(LOEL)	
Actual dose received by dose level and sex	
Parental data and F1 as appropriate	
Offspring toxicity F1 and F2	
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	No effect on early deaths, late fetal deaths and total implantations was reported when 2-isopropyl-5-methylcyclohexanol was administered to male rats prior to mating.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Food and Drug Administration (FDA) (1975) Mutagenic evaluation of compound FDA 71-57, menthol. NTIS PB-245-444 (FDA 71-268).
CAS	823-55-2
Substance Name	2,4-Dimethylcyclohexanone
Remarks for Substance	Data are for alkyl-substituted cyclohexanol, 2-Isopropyl-5-methylcyclohexanol
Method/guideline	
Test Type	Dominant lethal assay- Subacute study
GLP	No
Year	1975
Species/Strain	Random bred rat
Sex	Male
Route of administration	Oral-Gavage
Duration of test	
Doses/concentration levels	Test 1: 1.45, 14.5, or 145 mg/kg bw; test 2: 1150 mg/kg bw
Premating Exposure period	

for males	
Premating Exposure period for females	
Frequency of treatment	Five doses 24 hours apart
Control Group and treatment	Saline
Remarks for test conditions	Groups of rats were gavaged with 1.45, 14.5 or 145 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 1) or 1150 mg 2-isopropyl-5-methylcyclohexanol/kg bw (test 2) for 5 consecutive doses, 24 hours apart . After the last dose, male rats were mated with 2 female rats per week for 7 weeks. 14 days after mating, females were killed and the uterus was examined for early deaths, late fetal deaths and total implantations.
NOAEL(NOEL)	
LOAEL(LOEL)	
Actual dose received by dose level and sex	
Parental data and F1 as appropriate	
Offspring toxicity F1 and F2	
Appropriate statistical evaluations	
Remarks for results	
Conclusion remarks	No effect on early deaths, late fetal deaths and total implantations was reported when 2-isopropyl-5-methylcyclohexanol was administered to male rats prior to mating.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Food and Drug Administration (FDA) (1975) Mutagenic evaluation of compound FDA 71-57, menthol. NTIS PB-245-444 (FDA 71-268).

CAS	2345-28-0
Substance Name	2-Pentadecanone
Remarks for Substance	Substance identified by infrared and chemical assay performed by gas chromatography
Test Type	Fertility screening assay
GLP	No
Year	1975

Species/Strain	Mice/CF1
Sex	Female
Route of administration	Intraperitoneal
Duration of test	Period of gestation
Doses/concentration levels	50 mg/kg bw/day
Premating Exposure period for males	
Premating Exposure period for females	
Frequency of treatment	Daily
Control Group and treatment	62 untreated CF1 female mice
Remarks for test conditions	A group of 8 female CF1 mice were given 50 mg/kg bw dose of 2-pentadecanone by Intraperitoneal injection daily during gestation. The percent pregnant, number of viable fetuses per litter, number of resorption sites, and dead *in utero* per litter were recorded and expressed as a percent of the control value.
NOAEL(NOEL)	50 mg/kg bw
LOAEL(LOEL)	
Actual dose received by dose level and sex	50 mg/kg bw
Parental data and F1 as appropriate	No effect on maternal body weights was observed and no signs of toxicity were recorded. For the test group compared to the control group, 100% pregnancy rate, 0% for the average number of resorption sites per litter and 78% average number of fetuses per litter were reported. A 25% (p=0.05) difference between test and control group was considered significant by the authors. Diethylstilbesterol was used as a positive control (10 ug/kg bw). The positive control showed 0% pregnancy rate, 0% fetuses per litter, and 0% resorption sites per litter.
Offspring toxicity F1 and F2	
Appropriate statistical evaluations	Yes
Remarks for results	
Conclusion remarks	Under conditions of the experiment, a 50 mg/kg bw dose of 2-pentadecanone given daily by intraperitoneal injection to female rats produced no maternal or reproductive effects.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.

References	Carlson G. L., Hall I. H., and Piantadosi (1975) Cycloalkanone. 7. Hypocholesterolemic activity of aliphatic compounds related to 2,8-dibenzylcyclooctanone. Journal of Medicinal Chemistry 18(10), 234-236.
CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Substance identified by infrared and chemical assay performed by gas chromatography
Test Type	Fertility screening assay
GLP	No
Year	1975
Species/Strain	Mice/CF1
Sex	Female
Route of administration	Intraperitoneal
Duration of test	Period of gestation
Doses/concentration levels	50 mg/kg bw/day
Premating Exposure period for males	
Premating Exposure period for females	
Frequency of treatment	Daily
Control Group and treatment	62 untreated CF1 female mice
Remarks for test conditions	A group of 8 female CF1 mice were given 50 mg/kg bw dose of 2-undecanone by Intraperitoneal injection daily during gestation. The percent pregnant, number of viable fetuses per litter, number of resorption sites, and dead in utero per litter were recorded and expressed as a percent of the control value.
NOAEL(NOEL)	50 mg/kg bw
LOAEL(LOEL)	
Actual dose received by dose level and sex	50 mg/kg bw
Parental data and F1 as appropriate	No effect on maternal body weights was observed and no signs of toxicity were recorded. For the test group compared to the control group, 100% pregnancy rate, 0% for the average number of resorption sites per litter and 78% average number of fetuses per litter were reported. A 25% (p=0.05) difference between test and control group was considered significant by the authors. Diethylstilbesterol was used as a positive control (10 ug/kg bw). The positive control showed 0% pregnancy rate, 0% fetuses per

	litter, and 0% resorption sites per litter.
Offspring toxicity F1 and F2	
Appropriate statistical evaluations	Yes
Remarks for results	
Conclusion remarks	Under conditions of the experiment, a 50 mg/kg bw dose of 2-undecanone given daily by intraperitoneal injection to female rats produced no maternal or reproductive effects.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Carlson G. L., Hall I. H., and Piantadosi (1975) Cycloalkanone. 7. Hypocholesterolemic activity of aliphatic compounds related to 2,8-dibenzylcyclooctanone. Journal of Medicinal Chemistry 18(10), 234-236.

4.5 Developmental Toxicity

CAS	123-18-2
Substance Name	2,6,8-Trimethyl-4-nonanone
Remarks for Substance	Assay:>91%
Method/guideline	EPA OPPTS 370.3700, Prenatal Developmental Toxicity Study
Test Type	
GLP	Yes
Year	2002
Species/Strain	Rat/Sprague-Dawley
Sex	Female
Route of administration	Oral/gavage
Duration of test	Days 6-20 of gestation
Doses/concentration levels	250, 500, 750 or 1000 mg/kg/day
Exposure period	14 days
Frequency of treatment	Daily
Control Group and treatment	Controls were exposed to filtered room air and housed similarly.
Remarks for test conditions	Groups (8/group) of sexually mature adult female CD rats of age 10-11 weeks and weight 200-250g were given doses of 0,

	250, 500, 750 and 1000 mg IBHK/kg/day. IBHK in a 0.5% METHOCEL suspension by gavage daily for days 6-20 of gestation. Samples were analyzed to confirm concentration, stability and homogeneity During the study clinical observations were conducted daily throughout the study period. Maternal body weights were recorded on GD 0 (at the supplier), 3, 6, 9, 12, 15, 18 and 21. Food consumption data was recorded on GD 3-6, 6-9, 9-12, 12-15, 15-18 and 18-21. At conclusion of the study, all animals were submitted for a complete necropsy on day 21. The eyes were examined by visual inspection. Weights of the liver and kidneys were recorded and organ to body ratios calculated. Sections of liver, kidneys and gross lesions were preserved. - Examination of uterus: An examination of the uterus for the number of implantation sites and resorptions, and the ovaries for the number corpora lutea was performed. The position and number of early and/or late resorptions and normally developing fetuses were recorded. Corpora lutea for non-pregnant animals were not counted. The uteri of animals lacking visual implantations were stained and examined for evidence of early resorptions to verify pregnancy status
NOAEL (NOEL) maternal toxicity	The no-observed-adverse-effect level (NOAEL) for maternal toxicity was 250 mg/kg/day.
LOAEL (LOEL) maternal toxicity	500 mg/kg/day
NOAEL (NOEL) developmental toxicity	1000 mg/kg/day was considered a no-observed-effect-level (NOEL) for embryo/fetal toxicity.
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	
Maternal data with dose level	There were no maternal deaths during the study. Oral administration of IBHK resulted in increased salivation at all dose levels. Increased salivation was observed in all animals (8/8 each) in the 500-1000 mg/kg/day doses, whereas only 5 of 8 animals in the 250 mg/kg/day group exhibited this sign. Salivation was transient, usually ending within one hour of dosing, suggesting a local response to the taste of the test material. One dam delivered early in the 250 mg/kg/day dose group. Other clinical signs included a palpable mass on a dam in the 250 mg/kg/day dose level, which was identified as a firm mass-nodule on the left side of the neck at necropsy. Perineal urine soiling was noted in one animal in the 500 mg IBHK/kg/day group on gestation day 20 and a dam in the 750 mg/kg/day was observed with red vulvular discharge on gd 18. As these signs appeared as isolated incidences, they were not attributed to IBHK treatment. Exposure to 750 or 1000 rng IBHK/kg/day resulted in a decrease in body weight gains, 10 and 11% respectively, although these decrease were not significant. There were no significant differences in feed consumption between control and test animals Doses of 750 and t000 mg IBHK/kg/day produced statistically significant increases in absolute (28 and 33%) and relative liver

weights (30 and 33%). Relative liver weight was also significantly increased at 500 mg/kg/day (16%). There was a 14% increase in absolute liver weight at 500 mg/kg/day that was considered treatment-related, but not statistically significant. Mean relative kidney weight was significantly increased by 19% and absolute kidney weight was increased by 15%, not statistically significant, at the 1000 mg/kg/day dose level. There were no treatment-related gross pathologic observations.

For measured reproductive parameters, reproductive effects were at or above maternally toxic dose levels. There were no significant treatment-related effects on pregnancy rates, number ol corpora lutea, implantations, resorptions per litter with resorptions, or litter size. Mean percent post-implantation loss was significantly increased at 1000 mg/kg/day. An increase in the number of resorptions per litter was observed in the 1000 mg/kg/day dose, but the increase was not statistically significant and there was not a related decrease in the number of viable fetuses as compared to control. A significant decrease in mean percentage pre-implantation loss was seen at 1000 mg/kg/day, but a decrease in this parameter is not considered adverse.

Dose (mg/kg/day)	0	250	500	750	1000
Number Bred	6	8	8	8	8
# Pregnant	8/8	8/8	8/8	7/8	8/8
# Deaths	0	0	0	0	0
# Moribund	0	0	0	0	0
# Aborted	0	0	0	0	0
# Delivered Early	0	1	0	0	0

Fetal data with dose level

There were no treatment-related changes in pup clinical signs, weight gain, or abnormalities compared to controls at any of the test concentrations.

Appropriate statistical evaluations?

Maternal body weights, body weight gains, organ weights and feed consumption were evaluated by Bartlett's test for equality of variances. Based on the results, a parametnc or nonparametric analysis of variance (ANVOA) was performed. If the ANOVA was significant at alpha=0.05, analysis by Dunnett's Test or the Wilcoxon Rank Sum Test with Bonferroni's correction was performed.

Frequency of pre-implantation loss, post-implantation loss, resorptions per litter and resorptions per fetal population were analyzed using a Censored Wilcoxon Test with Bonferroni's correction. The number of corpora lutea and implantations, and litter size were evaluated using a nonparametric ANOVA followed by the Wilcoxon Rank-Sum Test with Bonferroni's correction. Pregnancy rates were analyzed using the Fisher exact probability Test with Bonferroni's correction. Non-pregnant females, females with resorptions only, or females found to be pregnant after staining of their uteri were excluded from the appropriate analyses. Statistical outliers were

	identified using a sequential method and excluded if justified by sound reason.
Remarks for results	
Conclusion remarks	The no-observed-adverse-effect level (NOAEL) for maternal toxicity was 250 mg/kg/day while 1000 mg/kg/day was considered a no-observed-effect-level (NOEL) for embryo/fetal toxicity.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Dow Chemical (2002) OECD Guideline No. 422, A Combined repeated dose toxicity study with the reproduction/ developmental toxicity screening test with 2,6,8-trimethyl-4-nonanone. Unpublished Report.
CAS	821-55-6
Substance Name	2-Nonanone
Remarks for Substance	Data are for structurally related substance 2-heptanone, purity greater than 99%.
Method/guideline	OECD:TG- 421
Test Type	
GLP	Yes
Year	2001
Species/Strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of administration	Inhalation
Duration of test	Males were exposed for 50 days; females were exposed for 34-47 days (through day 19 of gestation)
Doses/concentration levels	0, 80, 400, or 1000 ppm. Actual exposure concentrations 0, 78.6, 405.8 or 1022.6 ppm
Exposure period	6 hours/day
Frequency of treatment	7 days/week
Control Group and treatment	Controls were exposed to filtered room air and housed similarly.
Remarks for test conditions	The ovaries, vagina, uterus, Fallopian tubes, and testes, epididymis, and male accessory sex organs were examined histologically. The testes and epididymis were also weighed. The study design also included an analysis of epididymal spermatozoan numbers and motility, and testicular spermatid head counts.
NOAEL (NOEL) maternal toxicity	80 ppm

LOAEL (LOEL) maternal toxicity	400 ppm based on a reduction in activity
NOAEL (NOEL) developmental toxicity	1000 ppm
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	
Maternal data with dose level	All adult animals survived to study termination and there were no test substance-related changes in mean terminal body weight. For the 1000 ppm male group, there was a reduction in food consumption during days 0-7. Otherwise, there were no other differences in mean body weight, body weight gain, food consumption or food utilization among the groups throughout the study. Except for minimal reductions in activity level observed in the 400 and 1000 ppm groups during each exposure, no other test substance-related clinical abnormalities were noted. Mean sperm motility and mean epididymal spermatozoan and testicular spermatid counts were comparable among the groups. No test substance-related gross pathology was observed for adult animals from any group. No exposure-related changes were observed during histological examination of the reproductive organs of any of the test substance-exposed animals.
Fetal data with dose level	There were no treatment-related changes in pup clinical signs, weight gain, or abnormalities compared to controls at any of the test concentrations.
Appropriate statistical evaluations?	Homogeneity of data were evaluated by Bartlett's test (p,0.01), analysis of variance (ANOVA, <0.05), and Dunnett's test (p,0.05). When the variances of the means were not considered equal by Bartlett's test, the data were evaluated by Kruskal-Wallis H-test (p,0.05) followed by Mann-Whitney U-test (p<0.05). The reproductive performance of dams and fertility and fecundity indices were evaluated in contingency tables, using Chi-square test (p,0.05). The total number of pups per litter (live and dead) and the total number of live pups per litter were evaluated by a linear regression model.
Remarks for results	
Conclusion remarks	Test material did not induce reproductive or developmental toxicity under the conditions of this assay at exposure levels up to 1000 ppm.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Eastman Kodak Co. (1996) Reproduction/Developmental toxicity screening test in the rat. Toxicological Sciences Laboratory, Health and Environment Laboratories. Study No. HAEL 95-0202.

CAS	112-12-9
Substance Name	2-Undecanone
Remarks for Substance	Data are for structurally related substance, 6,10-dimethyl-2-undecatrienone, purity greater than 98% by HPLC.
Method/guideline	Experimental/Retinoid Teratogenicity
Test Type	Developmental Toxicity
GLP	No
Year	1986
Species/Strain	Hamster/Golden Syrian
Sex	Female
Route of administration	Oral-Gavage
Duration of test	14 days (days 1 to 14 of pregnancy)
Doses/concentration levels	0, 96, or 960 mg/kg
Exposure period	days 1-14 of pregnancy
Frequency of treatment	Single high dose level on Day 8 of pregnancy
Control Group and treatment	Control group received Tween 20 (0.5 ml/100g)
Remarks for test conditions	Timed pregnant LAK:LVG(SYR) hamsters were given the test material dissolved in acetone and solubilized in polyoxyethylene sorbitan monolaurate. The test material was administered by gavage. Fetal and maternal body weights were monitored on Day 14. Full batteries of developmental parameters were monitored. Pregnant uteri were collected after laparatomy. The numbers of resorption and dead fetuses were recorded. Live fetuses were weighed and one-third of each litter was fixed in Bouin's fluid and subsequently sectioned in the mid-sagittal plane. Two-thirds of each litter were processed for skeletal examination. Abnormal litters were those containing one or more malformed fetuses or three or more resorbed implantation sites.
NOAEL (NOEL) maternal toxicity	96 mg/kg
LOAEL (LOEL) maternal toxicity	960 mg/kg
NOAEL (NOEL) developmental toxicity	960 mg/kg
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	
Maternal data with dose level	Maternal body weight was significantly depressed at 960 mg/kg. There were no significant changes in any other maternal

	parameter monitored.
Fetal data with dose level	There were no significant changes in any fetal parameter and no malformations were observed at either dose level.
Appropriate statistical evaluations?	Fetal and maternal body weight data analyzed by Neman-Keuls test, number of absorptions by Mann-Whitney test, and number of litters by Yates X2 test.
Remarks for results	There was no evidence of maternal toxicity at 96 mg/kg and no evidence of developmental toxicity at 960 mg/kg in golden Syrian hamsters.
Conclusion remarks	
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Basic data given: comparable to guidelines/standards.
References	Willhite C. C. (1986) Structure-activity relationships of retenoids in developmental toxicology. II Influence of polyene chain of the Vitamin A molecule. Toxicology and Applied pharmacology, 83, 563-575.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related ketone 3,5,5-trimethylcyclohexenone, assay 96.8%.
Method/guideline	
Test Type	Inhalation teratology study
GLP	No
Year	1984
Species/Strain	Rat/Sprague Dawley
Sex	Female
Route of administration	Inhalation
Duration of test	6 hrs/day for days 6 through 15 of gestation
Doses/concentration levels	0, 25, 50, or 115 ppm
Exposure period	Days 6 to 15 of pregnancy
Frequency of treatment	Daily
Control Group and treatment	Control group received conditioned air.
Remarks for test conditions	Groups of pregnant female Fischer F344 rats (22/group, 11 weeks old) were exposed to atmospheres containing 0, 25, 50, or 115 ppm of 3,5,5-trimethyl-2-cyclohexenone 6 hours daily from days 6 to 15 of pregnancy. Rats were weighted on days 0, 3, 6, 9, 12, 15, 18, or 20 of the study. Food consumption was

	measured for the same three day intervals. Dams were sacrificed on Day 20 and the intact uteri with ovaries were weighed. The uterus was examined for live and dead fetuses and late and early resorptions. The stained uterus of each animal was examined for implantation site and Corpora lutea were counted. Live and dead fetuses were weighed, examined for abnormalities, and crown rump distance was measured. One half the fetuses from each litter were decapitated and the heads were preserved, sectioned and examined (Wilson's technique). The viscera of all fetuses were processed, staine (Alizarin Red) and examined. Fetuses that have no been decapitated were examined for skeletal malformations and ossification variations. Late resorptions were weighed and examined grossly. Three animals of each sex were selected prior to the study and 6 females at conclusion of the study were selected. These animals were subjected to necropsy, gross examination, and viral blood examination. A wide variety of tissues were taken grossly examined.
NOAEL (NOEL) maternal toxicity	115 ppm
LOAEL (LOEL) maternal toxicity	
NOAEL (NOEL) developmental toxicity	115 ppm
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	
Maternal data with dose level	There were deaths during the study. Mean body weights of the high exposure group were depressed on days 12-15 compared to controls. This correlated with decreased food consumption during days 6 to 20. Clinical observations included a dose-related alopecia and cervical and ano-genital staining. There were no significant differences in mean uterine implantation and fetal evaluation data between test and control groups. At necropsy, there were no significant abnormalities reported in any treatment or control group animals.
Fetal data with dose level	The incidence of malformations (fusion of the malar and maxillary or processes of the jaw) were similar for test and control animals. No significant differences were reported in the mean body weights and mean crown-rump distances between test and control animals.
Appropriate statistical evaluations?	Bartlett's test for homogeneity of variance was used to determine if test and control groups showed equivalent variance at the 1% level of significance. If variances were significant a linear regression was performed. To test for dose response Duncan's test was perfomed. If variances were not equivalent, non-parameteric analysis was performed with a Kruskal-Wallis test.
Remarks for results	

Conclusion remarks	Under conditions of the test, dose levels of 0,25, 50, or 115 ppm of 3,5,5-trimethyl-2-cyclohexenone were not fetotoxic or teratogenic.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Traul K.A. (1984) Inhalation teratology study in mice and rats. Biodynamics Inc. Project No. 323772. Unpublished report.
CAS	2979-19-3
Substance Name	3,3-Dimethylcyclohexanone
Remarks for Substance	Data are for structurally related ketone 3,5,5-trimethylcyclohexenone, assay 96.8%
Method/guideline	
Test Type	Inhalation teratology study
GLP	No
Year	1984
Species/Strain	Mice/CD-1
Sex	Female
Route of administration	Inhalation
Duration of test	6 hrs/day for days 6 through 15 of gestation
Doses/concentration levels	0, 25, 50, or 115 ppm
Exposure period	Days 6 to 15 of pregnancy
Frequency of treatment	Daily
Control Group and treatment	Control group received conditioned air.
Remarks for test conditions	Groups of pregnant female CD-1 mice (22/group, 9 weeks old) were exposed to atmospheres containing 0, 25, 50, or 115 ppm of 3,5,5-trimethyl-2-cyclohexenone 6 hours daily from days 6 to 15 of pregnancy. Mice were weighted on days 0, 3, 6, 9, 12, 15, and 18, of the study. Food consumption was measured for the same three day intervals. Dams were sacrificed on Day 18 and the intact uteri with ovaries were weighed. The uterus was examined for live and dead fetuses and late and early resorptions. The stained uterus of each animal was examined for implantation site and Corpora lutea were counted. Live and dead fetuses were weighed, examined for abnormalities, and crown rump distance was measured. One half the fetuses from each litter were decapitated and the heads were preserved, sectioned and examined (Wilson's technique). The viscera of all fetuses were processed, staine (Alizarin Red) and examined. Fetuses that have no been decapitated were examined for

	skeletal malformations and ossification variations. Late resorptions were weighed and examined grossly. Three animals of each sex were selected prior to the study and 6 females at conclusion of the study were selected. These animals were subjected to necropsy, gross examination, and viral blood examination. A wide variety of tissues were taken grossly examined.
NOAEL (NOEL) maternal toxicity	115 ppm
LOAEL (LOEL) maternal toxicity	
NOAEL (NOEL) developmental toxicity	115 ppm
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	
Maternal data with dose level	There were deaths during the study. Mean body weights of the high exposure group were depressed compared to controls. There were no significant differences in mean uterine implantation and fetal evaluation data between test and control groups. At necropsy there was no significant abnormalities reported in any treatment or control group animals.
Fetal data with dose level	The predominant skeletal malformation was an extra area of ossification between the frontal bones of the head. However, there were no significant differences between test and control groups. There were no significant differences in the mean body weights and mean crown-rump distances between test and control animals.
Appropriate statistical evaluations?	Bartlett's test for homogeneity of variance was used to determine if test and control groups showed equivalent variance at the 1% level of significance. If variances were significant a linear regression was performed. To test for dose response Duncan's test was perfomed. If variances were not equivalent, non-parameteric analysis was performed with a Kruskal-Wallis test.
Remarks for results	
Conclusion remarks	Under conditions of the test, dose levels of 0, 25, 50, or 115 ppm of 3,5,5-trimethyl-2-cyclohexenone were not fetotoxic or teratogenic.
Data Qualities Reliabilities	Reliability code 2. Reliable with restriction.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Traul K.A. (1984) Inhalation teratology study in mice and rats. Biodynamics Inc. Project No. 323772. Unpublished report.
CAS	2816-57-1

Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Based on inconvertibility of alcohol and ketones in vivo, data for structurally related alcohols 2-Isopropyl-5-methylcyclohexanol are presented.
Method/guideline	
Test Type	Teratology study
GLP	Pre-GLP
Year	1973
Species/Strain	Mouse/CD-1 outbred
Sex	Female
Route of administration	Gavage
Duration of test	10 days
Doses/concentration levels	0(negative control), 0, 1.85, 8.59, 39.9, 185 mg/kg bw/day and a positive control of 150 mg/kg bw/day of aspirin.
Exposure period	Days 6 to 15 of gestation
Frequency of treatment	Daily
Control Group and treatment	Control group received corn oil vehicle (10 ml//kg); Positive control received 150 mg/kg bw/day of aspirin in corn oil
Remarks for test conditions	Study measured parameters for reproductive and developmental toxicity. In the study, virgin adult female CD-1 outbred mice were gang-housed in plastic disposable cages in a temperature- and humidity-controlled room. Animals were given free access to food and fresh tap water. There were mated with untreated young adult males and observation of vaginal sperm plugs was considered day 0 of gestation. Beginning on Day 6 and continuing daily through Day 15 of gestation, groups (22-23/group) of pregnant females were given 0, 1.85, 8.59, 39.9, 185 mg/kg bw of the test material (FDA 71-57) by gavage in corn oil. A positive control group received 150 mg/kg bw/day of aspirin. Body weights were recorded on days 0, 6, 11, 15, and 17 of gestation. Females were observed daily for appearance and behavior. Food consumption and body weight were monitored to eliminate any abnormalities that may be associated with anorexia in pregnant females. On Day 17 all dams were subjected to Caesarean section and the number of implantation sites, number of resorptions, % of live and % partial live resorptions, live fetuses, dead fetuses, and body weight of live pups were recorded. Gestation index, mortality, litter size and weights, sex and sex ratio of pups, and gross abnormalities to pups were reported. The urogenital tract of each dam was examined for anatomical abnormalities. One-third of fetuses of each litter underwent detailed visceral examination at 10x magnification. The remaining two-thirds were stained with alizarin red S dye/KOH and examined for skeletal defects.

NOAEL (NOEL) maternal toxicity	185 mg/kg bw/day
LOAEL (LOEL) maternal toxicity	
NOAEL (NOEL) developmental toxicity	185 mg/kg bw/day
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	0, 1.85, 8.59, 39.9, 185 mg/kg bw of the test material (FDA 71-57)
Maternal data with dose level	Daily clinical observation and measurement of body weight gain failed to show any differences between control and test groups of female mice. The number pregnant and % pregnancy were similar for all dose and control groups. No abortions were observed in any group. The number of live litters, average implant sites per dam were similar for both test and control groups. The % partial resorptions and % complete resorption were increased for the 1.85 and 8.59 mg/kg bw groups, but higher dose levels exhibited lower resorption rates compared to the control groups.
Fetal data with dose level	The average fetal weight of treatment and control groups were not statistically different ($p>0.05$). The total number of live fetuses was similar for test and control groups. Also, there was no significant difference in the number of dead fetuses between test and control groups. Skeletal examination of sternebrae showed no significant differences in the incidence of incomplete ossification or missing sternebrae for test and negative control groups. There was evidence of incomplete ossification in the positive control group. Likewise the incidences of fetuses with more than 13 ribs, incomplete ossification of vertebrae and extremities, incomplete skull closure were similar for test and negative control animals. Visceral examination failed to reveal any evidence of soft tissue abnormalities at any dose level.
Appropriate statistical evaluations?	
Remarks for results	
Conclusion remarks	There was no evidence of maternal toxicity or developmental toxicity at dose levels up to and including 185 mg/kg bw/day of test material.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Morgareidge K. (1973a) Teratologic evaluation of FDA 71-57 in mice. Contract No. FDA 71-260. Unpublished report.
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone

Remarks for Substance	Based on inconvertibility of alcohol and ketones in vivo, data for structurally related alcohols 2-Isopropyl-5-methylcyclohexanol are presented.
Method/guideline	
Test Type	Teratology study
GLP	Pre-GLP
Year	1973
Species/Strain	Rat/female Wistar
Sex	Female
Route of administration	Gavage
Duration of test	10 days
Doses/concentration levels	0(control), 2.18, 10.15, 47.05, 218 mg/kg bw/day and a positive control of 250 mg/kg bw/day of aspirin in corn oil.
Exposure period	Days 6 to 15 of gestation
Frequency of treatment	Daily
Control Group and treatment	Control group received corn oil vehicle (10 ml//kg); Positive control received 250 mg/kg bw/day of aspirin in corn oil
Remarks for test conditions	Study measured parameters for reproductive and developmental toxicity. In the study, virgin adult female rats were individually housed in mess bottom cages in a temperature- and humidity-controlled room. Animals were given free access to food and fresh tap water. There were mated with untreated young adult males and observation of vaginal sperm plugs was considered day 0 of gestation. Beginning on Day 6 and continuing daily through Day 15 of gestation, groups (22-25/group) of pregnant females were given 0, 2.18, 10.15, 47.05, 218 mg/kg bw of the test material (FDA 71-57) by gavage in corn oil. A positive control group received 250 mg/kg bw/day of aspirin. Body weights were recorded on days 0, 6, 11, 15, and 20 of gestation. Females were observed daily for appearance and behavior. Food consumption and body weight were monitored to eliminate any abnormalities that may be associated with anorexia in pregnant females. On Day 20 all dams were subjected to Caesarean section and the number of implantation sites, number of resorptions, % of live and % partial live resorptions, live fetuses, dead fetuses, and body weight of live pups were recorded. Gestation index, mortality, litter size and weights, sex and sex ratio of pups, and gross abnormalities to pups were reported. The urogenital tract of each dam was examined for anatomical abnormalities. One-third of fetuses of each litter underwent detailed visceral examination at 10x magnification. The remaining two-thirds were stained with alizarin red S dye/KOH and examined for skeletal defects.
NOAEL (NOEL) maternal toxicity	218 mg/kg bw/day

LOAEL (LOEL) maternal toxicity	
NOAEL (NOEL) developmental toxicity	218 mg/kg bw/day
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	0, 2.18, 10.15, 47.05, 218 mg/kg bw of the test material (FDA 71-57)
Maternal data with dose level	Daily clinical observation and measurement of body weight gain failed to show any differences between control and test groups of female rats. The number pregnant and % pregnancy were similar for all dose and control groups. No abortions were observed in any group. The number of live litters, average implant sites per dam were similar for both test and control groups. The % partial resorptions and % complete resorption were increased only for the positive control group.
Fetal data with dose level	The average fetal weight of treatment and control groups were not statistically different ($p>0.05$). The total number of live fetuses was similar for test and negative control groups. Also, there no dead fetuses in either the test or negative control groups. The positive control group did show dead fetuses (3) and dams with more than one dead fetus. The positive control group also exhibited a decreased number of live fetuses and decreased average fetal weight compared to those for the negative control. Skeletal examination of sternebrae, vertebrae, skull, ribs, extremities, and soft tissues showed no significant differences between test and negative control groups. The positive control group showed a significant increase in incidence of missing sternebrae. Likewise, the positive control exhibited an increase in the incidence of fetuses with more than 13 ribs, incomplete ossification of vertebrae and extremities, incomplete skull closure. Visceral examination failed to reveal any evidence of abnormalities in either negative control or test groups. In the positive control group, meningoencephalocele and spina bifida were reported.
Appropriate statistical evaluations?	
Remarks for results	
Conclusion remarks	There was no evidence of maternal toxicity or developmental toxicity at dose levels up to and including 218 mg/kg bw/day of test material.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Morgareidge K. (1973b) Teratologic evaluation of FDA 71-57 in rats. Contract No. FDA 71-260. Unpublished report.
CAS	2816-57-1

Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Based on inconvertibility of alcohol and ketones in vivo, data for structurally related alcohols 2-Isopropyl-5-methylcyclohexanol are presented.
Method/guideline	
Test Type	Teratology study
GLP	Pre-GLP
Year	1973
Species/Strain	Hamster/female golden
Sex	Female
Route of administration	Gavage
Duration of test	5 days
Doses/concentration levels	0(control), 4.05, 21.15, 98.2, or 405 mg/kg bw/day and a positive control of 250 mg/kg bw/day of aspirin
Exposure period	Days 6 to 10 of gestation
Frequency of treatment	Daily
Control Group and treatment	Control group received corn oil vehicle (10 ml//kg); Positive control received 250 mg/kg bw/day of aspirin in corn oil
Remarks for test conditions	Study measured parameters for reproductive and developmental toxicity. In the study, virgin adult female hamsters were individually housed in mess bottom cages in a temperature- and humidity-controlled room. Animals were given free access to food and fresh tap water. There were mated one to one with untreated young adult males and the appearance of motile sperm in the vaginal sperm was considered day 0 of gestation. Beginning on Day 6 and continuing daily through Day 10 of gestation, groups (19-23/group) of pregnant females were given 0, 64.05, 21.15, 98.2, or 405 mg/kg bw of the test material (FDA 71-57) by gavage in corn oil. A positive control group received 250 mg/kg bw/day of aspirin. Body weights were recorded on days 0, 8, 10, and 14 of gestation. Females were observed daily for appearance and behavior. Food consumption and body weight were monitored to eliminate any abnormalities that may be associated with anorexia in pregnant females. On Day 14 all dams were subjected to Caesarean section and the number of implantation sites, resorption sites, % of live and % partial live resorptions, live fetuses, dead fetuses, and body weight of live pups were recorded. Gestation index, mortality, litter size and weights, sex and sex ratio of pups, and gross abnormalities to pups were reported. The urogenital tract of each dam was examined for anatomical abnormalities. One-third of fetuses of each litter underwent detailed visceral examination at 10x magnification. The remaining two-thirds were stained with alizarin red S dye/KOH and examined for skeletal defects.

NOAEL (NOEL) maternal toxicity	405 mg/kg bw/day
LOAEL (LOEL) maternal toxicity	
NOAEL (NOEL) developmental toxicity	405 mg/kg bw/day
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	0, 4.05, 21.15, 98.2, or 405 mg/kg bw of the test material (FDA 71-57)
Maternal data with dose level	Daily clinical observation and measurement of body weight gain failed to show any differences between control and test groups of female rats. The number pregnant and % pregnancy were similar for all dose and control groups. No abortions were observed in any group.
Fetal data with dose level	The average fetal weight of treatment and control groups were not statistically different ($p>0.05$). The total number of live fetuses was similar for test and control groups. There was one dead fetus in the negative control and the 4.05 and 21.15 dose groups, but none in the higher dose groups. There were 18 dead fetuses in the positive control group. Skeletal examination of sternebrae showed no significant differences in the incidence of incomplete ossification or missing sternebrae for test and control groups. Likewise the incidences of fetuses with more than 13 ribs, incomplete ossification of vertebrae and extremities, incomplete skull closure were similar for test and control animals. An increased incidence of incomplete ossification of the vertebrae was reported in the two mid-dose groups but not in the highest (405 mg/kg bw) group. Visceral examination of tissues failed to reveal any evidence of significant abnormalities at any dose level.
Appropriate statistical evaluations?	
Remarks for results	
Conclusion remarks	There was no evidence of maternal toxicity or developmental toxicity at dose levels up to and including 405 mg/kg bw/day of test material.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Morgareidge K. (1973c) Teratologic evaluation of FDA 71-57 in hamsters. Contract No. FDA 71-260. Unpublished report.
CAS	2816-57-1
Substance Name	2,6-Dimethylcyclohexanone
Remarks for Substance	Based on inconvertibility of alcohol and ketones in vivo, data for structurally related alcohols 2-Isopropyl-5-methylcyclohexanol

	are presented.
Method/guideline	
Test Type	Teratology study
GLP	Pre-GLP
Year	1973
Species/Strain	Rabbit/virgin, adult, Dutch belted
Sex	Female
Route of administration	Gavage
Duration of test	13 days
Doses/concentration levels	0(control), 4.25, 19.75, 91.7, 425 mg/kg bw/day and a positive control of 250 mg/kg bw/day of aspirin in corn oil.
Exposure period	Days 6 to 18 of gestation
Frequency of treatment	Daily
Control Group and treatment	Control group received corn oil vehicle (10 ml//kg); Positive control received 2.5 mg/kg bw/day of 6-aminonictineamide in corn oil on Day 9
Remarks for test conditions	Study measured parameters for reproductive and developmental toxicity. In the study, virgin adult female rabbits were individually housed in mess bottom cages in a temperature- and humidity-controlled room. Animals were given free access to food and fresh tap water. On day 0, does were given an injection of 0.4 l of human chorionic gonadotropin (400 IU). Three hours later, each doe was artificially inseminated with 0.3 ml of semen from a buck using approximately 20 x 10e6 motile sperm. Beginning on Day 6 and continuing daily through Day 18 of gestation, groups (11-14/group) pregnant females were given 0, 4.25, 19.75, 91.7, 425 mg/kg bw of the test material (FDA 71-57) by gavage in corn oil. A positive control group received 2.5 mg/kg bw/day of 6-aminonicotinamide. Body weights were recorded on days 0, 6, 8, 12, 18, and 29 of gestation. Females were observed daily for appearance and behavior. Food consumption and body weight were monitored to eliminate any abnormalities that may be associated with anorexia in pregnant females. On Day 29 all dams were subjected to Caesarean section and the number of corpora lutea, implantation sites, resorption sites, live fetuses, dead fetuses, and body weight of live pups were recorded. Gestation index, mortality, litter size and weights, sex and sex ratio of pups, and gross abnormalities to pups were reported. The urogenital tract of each dam was examined for anatomical abnormalities. All live fetuses were placed in an incubator for 24 hours and evaluated for survival. All surviving pups were sacrificed and subjected to detailed visceral examination at 10x magnification. All fetuses were cleared with KOH, stained with alizarin red S dye, and examined for skeletal defects.

NOAEL (NOEL) maternal toxicity	425 mg/kg bw/day
LOAEL (LOEL) maternal toxicity	
NOAEL (NOEL) developmental toxicity	425 mg/kg bw/day
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	0, 4.25, 19.75, 91.7, 425 mg/kg bw of the test material (FDA 71-57)
Maternal data with dose level	Survival of dams at term was similar for test, positive and negative control groups. Daily clinical observation and measurement of body weight gain failed to show any differences between control and test groups of female rabbits. The number pregnant and % pregnancy were similar for all dose and control groups. One to four pregnant female died in both control groups and in the four test groups. There was no dose response relationship for mortality in the test groups. There was no statistical difference in the number of live litters, corpora lutea, implantation sites, or resorption sites between the negative control group and any test group.
Fetal data with dose level	The average fetal weight of treatment and control groups were not statistically different ($p>0.05$). The total number of live fetuses was similar for test and control groups. Also, there was no significant difference in the number of dead fetuses between test and control groups. Except for positive control group, skeletal examination of sternebrae and vertebrae showed no significant differences in the incidence of incomplete ossification or missing sternebrae for test and untreated control group. Likewise the incidences of fetuses with more than 13 ribs, incomplete ossification of vertebrae and extremities, incomplete skull closure were similar for test and the untreated control group The positive 6-aminonicotinaminde-treated control group showed increases in incidence of fused and split ribs. Visceral examination failed to reveal any evidence of abnormalities in either negative control or test groups. In the positive control group, medial rotation of the hind limb and anopia were reported in pups from 7 of the 11 litters.
Appropriate statistical evaluations?	
Remarks for results	
Conclusion remarks	There was no evidence of maternal toxicity or developmental toxicity at dose levels up to and including 425 mg/kg bw/day of test material.
Data Qualities Reliabilities	Reliability code 2. Reliable with restrictions.
Remarks for Data Reliability	Code 2. Acceptable, well-documented publication/study report which meets basic scientific principles.
References	Morgareidge K. (1973d) Teratologic evaluation of FDA 71-57 in rabbits. Contract No. FDA 71-260. Unpublished report.

CAS	928-68-7
Substance Name	6-Methyl-2-heptanone
Remarks for Substance	Data are for structurally related substance 5-methyl-2-hexanone purity greater than 99%.
Method/guideline	OECD:TG- 421
Test Type	
GLP	Yes
Year	2001
Species/Strain	Rat/Sprague-Dawley
Sex	Male and Female
Route of administration	Inhalation
Duration of test	Males were exposed for 51 days; females were exposed for 35-41 days (through day 19 of gestation).
Doses/concentration levels	0, 1, 2.5, 5 mg/L. Actual exposure 0.965, 2.32, and 4.72 mg/L
Exposure period	6 hours/day
Frequency of treatment	7 days/week
Control Group and treatment	Controls were exposed to filtered room air and housed similarly.
Remarks for test conditions	The study design also included an analysis of epididymal spermatozoan numbers and motility, and testicular spermatid head counts.
NOAEL (NOEL) maternal toxicity	5 mg/L
LOAEL (LOEL) maternal toxicity	
NOAEL (NOEL) developmental toxicity	5 mg/L
LOAEL (LOEL) developmental toxicity	
Actual dose received by dose level and sex	
Maternal data with dose level	All adult animals survived to study termination and there were no test substance-related changes in mean terminal body weight. For the 5 mg/L male group, the mean body weight gain and mean food utilization were higher (p 0.05) on Day 35 when compared with the control group. Otherwise, there were no other differences in mean body weight, body weight gain, food consumption or food utilization among the groups throughout the study. Except for minimal reductions in activity level observed in the 5 mg/L group during each exposure, no other

	test substance-related clinical abnormalities were noted. Mean sperm motility and mean epididymal spermatozoan and testicular spermatid counts were comparable among the groups. No test substance-related gross pathology was observed for adult animals from any group. No exposure-related changes were observed during histological examination of the reproductive organs of any of the test substance-exposed animals.
Fetal data with dose level	Although trend analyses indicated reductions in the total number of pups per litter and in the number of live pups per litter. The Kruskal-Wallis H-test indicated that the total number of pups per litter and the number of live pups per litter were comparable among the groups. Abnormalities were observed for occasional pups from the 5.0, 2.5, and 0.0 mg/L groups. These abnormalities included the pups appearing small, having no milk in their stomachs, and having bruises under the skin. Additionally, pups were occasionally missing (presumable cannibalized) or found dead. Since the clinical abnormalities were observed for comparable numbers of pups from the control and treated groups and since the number of dead pups was not statistically different among the groups, these findings were not considered to be test substance-related.
Appropriate statistical evaluations?	
Remarks for results	
Conclusion remarks	Test material did not induce reproductive or developmental toxicity under the conditions of this assay at exposure levels up to 5 mg/L.
Data Qualities Reliabilities	Reliability code 1. Reliable without restriction.
Remarks for Data Reliability	Code 1. Guideline study.
References	Eastman Kodak Co. (2001b) Reproduction/Developmental toxicity screening test in the rat. Toxicological Sciences Laboratory, Health and Environment Laboratories. Study No. HAEL 2000-0208. Laboratory Project ID 200020818I1.